

To: Jan Delaval

Access DB# 91837

SEARCH REQUEST FORM

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Title of Invention: _____

Inventors (please provide full names): Tomikawa, Mayumi

Earliest Priority Filing Date: _____

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search claims 13-15. +
inventor's search.

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Thank you

Michael Borin

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Date Completed: <u>5/6/03</u>	Litigation _____	Lexis/Nexis _____
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Clerical Prep Time: <u>20</u>	Patent Family _____	WWW/Internet _____
Online Time: <u>+120</u>	Other _____	Other (specify) _____

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:58:15 ON 06 MAY 2003

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FILE COVERS 1907 - 6 May 2003 VOL 138 ISS 19

FILE LAST UPDATED: 5 May 2003 (20030505/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 19 all tot

L9 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2003 ACS

AN 2001:485453 HCAPLUS

DN 135:89486

TI Biopolymer model-generating apparatus and program-recording media

IN Aikawa, Ayako; Aikawa, Seiichi

PA Fujitsu Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 15 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

IC ICM G06F017-50

ICS C12M001-34; G01N033-50; G01N033-68

CC 9-1 (Biochemical Methods)

Section cross-reference(s): 6

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	-----	-----	-----
PI	JP 2001184376	A2	20010706	JP 1999-367353	19991224
PRAI	JP 1999-367353		19991224		

AB A biopolymer model-generating app. is provided for generating a homodimer model or a heterodimer model from the known biopolymer model (e.g., protein). Using this app., a biopolymer dimer is efficiently analyzed as for its structure such as interaction sites and its function. Diagrams describing the app. principle constitution, program-processing flow, and dimer models are given.

ST biopolymer model protein dimer app

IT Apparatus

Computer program

Memory devices

Simulation and Modeling, physicochemical

(biopolymer model-generating app. and program-recording media)

IT Biopolymers

Dimers

Proteins, general, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(biopolymer model-generating app. and program-recording media)

L9 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2003 ACS
 AN 1995:103134 HCAPLUS
 DN 122:125329
 TI Computerized system for automatic analysis of genetic information
 IN Tomikawa, Mayumi; Aikawa, Seiichi; Matsuzawa, Fumiko
 PA Fujitsu Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 13 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C12N015-09
 CC 3-1 (Biochemical Genetics)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06181765	A2	19940705	JP 1992-246558	19920916
PRAI	JP 1992-246558		19920916		

AB An automated system is described for the anal. of genetic information from the inputted DNA or amino acid sequences, or motif. The system is comprised of a DNA sequence database, amino acid sequence data base, motif database, LCS (longest common subsequence) detector, homol.-detg. subroutine, multiple alignment subroutine, motif extn. subroutine, etc.
 ST computer app automation gene analysis
 IT Computer application
 Information science and technology
 (computerized system for automatic anal. of genetic information)
 IT Gene
 RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
 (computerized system for automatic anal. of genetic information)

L9 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2003 ACS
 AN 1994:428600 HCAPLUS
 DN 121:28600
 TI Apparatus for automatic selection of restriction endonucleases for genetic engineering
 IN Matsuzawa, Fumiko
 PA Fujitsu Ltd, Japan
 SO Jpn. Kokai Tokkyo Koho, 13 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM G06F015-40
 ICA C12M001-00
 CC 3-1 (Biochemical Genetics)
 Section cross-reference(s): 7
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06096127	A2	19940408	JP 1992-242180	19920910
PRAI	JP 1992-242180		19920910		

AB An app. for automatic selection of appropriate restriction endonucleases for a DNA sequence contains a database of the recognition sites for each enzyme. A sample DNA sequence is compared with a selected enzyme to det. whether the restriction sites exist or the no. of the restriction sites. It can be used to select an enzyme that has the closest restriction sites to a gene by screening the enzymes that have restriction sites upstream and downstream. The length of a restriction fragment can also be predetd. by this method during cloning.
 ST restriction endonuclease automatic selection app
 IT Genetic methods
 (automatic, for selecting restriction endonucleases)
 IT Apparatus

(for automatic selection of restriction endonuclease, for genetic engineering)
IT 9075-08-5, Restriction endonuclease
RL: USES (Uses)
(app. for automatic selection of, for genetic engineering)

=> fil wpix
FILE 'WPIX' ENTERED AT 08:58:25 ON 06 MAY 2003
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FILE LAST UPDATED: 5 MAY 2003 <20030505/UP>
MOST RECENT DERWENT UPDATE: 200329 <200329/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

Due to data production problems in updates 24 and 25
the WPI file had to be reset to update 200323 on April 24
and the corrected updates were reloaded.
SDIs for update 24 were rerun. The previous SDI run for 24 has
been credited.
We also recommend to recreate answer sets dated between April 10
and 24. Charges incurred to accomplish this will be credited of
course.

>>> NEW WEEKLY SDI FREQUENCY AVAILABLE --> see NEWS <<<

>>> SLART (Simultaneous Left and Right Truncation) is now
available in the /ABEX field. An additional search field
/BIX is also provided which comprises both /BI and /ABEX <<<

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http://www.stn-international.de/training_center/patents/stn_guide.pdf <<<

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GUIDES, PLEASE VISIT:
http://www.derwent.com/userguides/dwpi_guide.html <<<

=> d 127 all abeq tech abex tot

L27 ANSWER 1 OF 7 WPIX (C) 2003 THOMSON DERWENT
AN 2002-712495 [77] WPIX
CR 1993-308303 [39]; 2002-487852 [52]; 2002-507172 [54]; 2002-607266 [65]
DNN N2002-562026
TI Atomic group sequence analysis method for medical research and
development, involves determining longest common atomic group between two
amino acid sequences based on character sequence occurrence table.
DC T01
IN AIKAWA, S; MATSUZAWA, F; TOMIKAWA, M
PA (FUIT) FUJITSU LTD
CYC 1
PI US 2002116146 A1 20020822 (200277)* 67p G06F017-18 <--
ADT US 2002116146 A1 Div ex US 1993-14867 19930208, US 2001-910071 20010723
PRAI JP 1992-331703 19921211; JP 1992-21012 19920206
IC ICM G06F017-18
AB US2002116146 A UPAB: 20021129
NOVELTY - Elements of an array S(i) corresponding to character sequence
are set to zero. Occurrence positions (r) of each character of a

subsequent sequence is determined from occurrence table indicative of positions of characters in the character sequence. $S(r)$ and $S(r-1)$ array are compared for each occurrence. The values of the array elements satisfying i at least r and $S(r) = S(r-1)$ are incremented so that $S(m)$ provides longest common subsequence (LCS).

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are included for the following:

- (1) a 3D structure analysis method;
- (2) an atomic group sequence analysis apparatus;
- (3) a 3D structure analysis apparatus.

USE - For evaluating mutually similar portions between amino acid sequences such as human cytochrome and bacteria cytochrome proteins of DNA in organism or between 3D structures of protein molecules and also for amino acids sequence of proteins such as calmodulin, troponin C, etc., for medical research and development.

ADVANTAGE - Enables efficient determination of homologous amino acids by determining LCS based on the character sequence of input amino acid. Hence, enables development of new medicines using improved functions.

DESCRIPTION OF DRAWING(S) - The figure shows a flowchart explaining atomic group sequence analysis process.
Dwg.3/47

FS EPI
FA AB; GI
MC EPI: **T01-J06A**

L27 ANSWER 2 OF 7 WPIX (C) 2003 THOMSON DERWENT

AN 2002-607266 [65] WPIX

CR 1993-308303 [39]; 2002-487852 [52]; 2002-507172 [54]; 2002-712495 [77]

DNN N2002-480864 DNC C2002-171643

TI Analysis of sequences of atomic groups for automatically extracting and evaluating mutually coinciding or similar portions between amino acid sequences in proteins, comprises obtaining a longest common atomic group number.

DC B04 D16 S03 T01

IN AIKAWA, S; MATSUZAWA, F; TOMIKAWA, M

PA (FUIT) FUJITSU LTD

CYC 1

PI US 2002072863 A1 20020613 (200265)* 65p G06F019-00 <--

ADT US 2002072863 A1 Div ex US 1993-14867 19930208, US 2001-909809 20010723

PRAI JP 1992-331703 19921211; JP 1992-21012 19920206

IC ICM G06F019-00

ICS G01N033-48

AB US2002072863 A UPAB: 20021204

NOVELTY - Sequences of atomic groups including first and second sequences having m and n atomic groups, respectively are analyzed by:

- (a) preparing an array $S(i)$ having array elements $S(0)$ to $S(m)$;
- (b) initializing all array elements of the array $S(i)$ to 0 and initializing an integer j to 1;
- (c) adding 1 to each array element and 1 to the integer j until j exceeds n ; and

- (d) obtaining a longest common atomic group number.

DETAILED DESCRIPTION - Analysis of sequences of atomic groups including first and second sequences respectively having m and n atomic groups comprises:

- (a) preparing an array $S(i)$ having array elements $S(0)$ to $S(m)$;
- (b) initializing all array elements of the array $S(i)$ to 0 and initializing an integer j to 1;
- (c) adding 1 to each array element $S(i)$ that is equal to an array element $S(r)$ and that i at least r if the array element $S(r)$ is equal to an array element $S(r-1)$, where r is an occurrence position of j -th atomic group of the second sequence in the first sequence, and adding 1 to the integer j , until j exceeds n ; and
- (d) obtaining a longest common atomic group number between the first

and second sequences from a value of the array element $S(m)$.

INDEPENDENT CLAIMS are included for the following:

(1) analyzing three-dimensional structures including a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, which comprises:

(a) dividing the first point set and second point set into first subsets and second subsets, respectively, according to a secondary structure exhibited by the three-dimensional coordinates of the elements of the first and second point sets;

(b) generating a combination of correspondence satisfying a first restriction condition between the first subsets and the second subsets from among candidates for the combination of correspondence;

(c) determining an optimum correspondence between the elements belonging to each pair of subsets corresponding in the combination of correspondence; and

(d) calculating a root mean square distance between all of the elements corresponding in the optimum correspondence;

(2) an apparatus for analyzing sequences of atomic groups, which comprises:

(i) a mechanism for preparing an array $S(i)$ having array elements $S(0)$ to $S(m)$;

(ii) a mechanism for initializing all array elements of the array $S(i)$ to zero and initializing an integer j to 1;

(iii) a mechanism for renewing the array $S(i)$ by adding 1 to each array element $S(i)$ that is equal to an array element $S(r)$ and that i at least r if the array element $S(r)$ is equal to an array element $S(r-1)$ where r is an occurrence position of j -th atomic group of the second sequence in the first sequence;

(iv) a mechanism for incrementing the integer j by 1;

(v) a mechanism for repeatedly activating the renewing mechanism and the incrementing mechanism until the integer j exceeds n ; and

(vi) a mechanism for obtaining a longest common atomic group number between the first and the second sequences from a value of the array element $S(m)$; and

(3) an apparatus for analyzing three-dimensional structures, which comprises:

(i) a mechanism for dividing the first point set and the second point set into first subsets and second subsets, respectively, according to a secondary structure exhibited by the three-dimensional coordinates of the elements of the first and second point sets;

(ii) a mechanism for generating a combination of correspondence satisfying a first restriction condition between the first subsets and the second subsets from among candidates for the combination of correspondence;

(iii) a mechanism for determining an optimum correspondence between the elements belonging to each pair of subsets corresponding in the combination of correspondence generated in the generating mechanism; and

(iv) a mechanism for calculating a root mean square distance between all of the elements corresponding in the optimum correspondence.

USE - The method is used for analyzing sequences of atomic groups, particularly for automatically extracting and evaluating mutually coinciding or similar portions between amino acid sequences in protein molecules and/or between three-dimensional structures of protein molecules.

ADVANTAGE - The invention prevents the generation of unnecessary combinations, thus allowing the points sets to be related efficiently.

DESCRIPTION OF DRAWING(S) - The figure shows a flowchart for a process for detecting a longest common character number in a longest common subsequence (LCS) detection unit.

Dwg. 2/47

FS CPI EPI
FA AB; GI; DCN

MC CPI: B04-N04; B11-C08E6; B11-C08F3; B12-K04; D05-H09; D05-H10
EPI: S03-E14H5; **T01-E01C**

TECH UPTX: 20021010

TECHNOLOGY FOCUS - BIOTECHNOLOGY - Preferred Method: The method of analyzing sequences of atomic groups further comprises:
(a) preparing an array data(k) having array elements data(0), data(1)...;
(b) storing paired data (r, j) in an array element data(k) if the array element S(i) is changed, where $k = S(r)$;
(c) linking the stored paired data (r, j) to paired data (r', j') if r' is less than r and j' is less than j, where the paired data (r', j') is one stored in an array element data (k-1);
(d) obtaining a longest common subsequence (LCS) between the first and second sequences and occurrence positions of the LCS in the first and second sequence by tracing the linked formed; evaluating homology between the first and second sequences based on the longest common atomic group number and a value of one of m and n; and
(e) searching for a sequence that is homologous with the first sequence from among several sequences by successively assigning one sequence to the second sequence and executing the first six steps of the method and evaluating the homology between the sequences.

The optimum correspondence determining step comprises:

(a) generating a combination of correspondence satisfying a second restricting condition between the elements belonging to the subsets corresponding in the combination of the correspondence generated;
(b) calculating a root mean square distance between the elements corresponding in the combination of the correspondence generated; and
(c) selecting a combination of the correspondence as the optimum correspondence according to the value of the root mean square distance value calculated.

L27 ANSWER 3 OF 7 WPIX (C) 2003 THOMSON DERWENT

AN 2002-507172 [54] WPIX

CR 1993-308303 [39]; 2002-487852 [52]; 2002-607266 [65]; 2002-712495 [77]

DNN N2002-401327 DNC C2002-144121

TI Analysis of three-dimensional structures by generating combination of correspondence satisfying restriction condition, and calculating root mean square distance between elements in the combination of correspondence.

DC B04 D16 S03 T01

IN AIKAWA, S; MATSUZAWA, F; TOMIKAWA, M

PA (FUJITSU) FUJITSU LTD

CYC 1

PI US 2002035434 A1 20020321 (200254)* 65p G06F017-60 <--

ADT US 2002035434 A1 Div ex US 1993-14867 19930208, US 2001-910054 20010723

PRAI JP 1992-331703 19921211; JP 1992-21012 19920206

IC ICM G06F017-60

ICS G01N031-00; G06F019-00

AB US2002035434 A UPAB: 20021204

NOVELTY - Analysis of three dimensional structures involves generating a combination of correspondence satisfying a restriction condition between the elements belonging to a first and second point sets from among all candidates for the combination of correspondence, and calculating a root mean square distance between the elements corresponding in the combination of correspondence.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are included for the following:

(1) a method of analyzing sequences of atomic groups including a first sequence having m atomic groups and a second sequence having n atomic groups;

(2) an apparatus for analyzing sequences of atomic groups; and

(3) an apparatus for analyzing three-dimensional structures.

USE - For analyzing three-dimensional structures of molecules, particularly protein molecules.

ADVANTAGE - The invention is capable of automatically extracting and

evaluating mutually coinciding or similar portions between three-dimensional structures of the molecules.

DESCRIPTION OF DRAWING(S) - The figure is a block diagram showing a construction of a gene information survey apparatus.

Dwg.1/47

FS CPI EPI

FA AB; GI; DCN

MC CPI: B04-C01; B04-N04; B11-C08F3; B11-C08F4; B12-K04E; D05-H09

EPI: S03-E14H5; S03-E15; **T01-J**; **T01-J05A**

TECH UPTX: 20020823

TECHNOLOGY FOCUS - INSTRUMENTATION AND TESTING - Preferred Parameters: The restriction condition includes order relation of the elements in the first and second point sets, proximity in a geometric relationship among elements close to each other, a condition so that a candidate for the combination of correspondence satisfies a threshold value condition, or a condition so that an attribute value of each element belonging to the first point set coincides with an attribute value of the corresponding element belonging to the second point set in a candidate for a combination of correspondence.

Preferred Method: The method of analyzing sequences of atomic groups involves preparing an array S(i) having array elements S(0) to S(m). All array elements of the array S(1) are initialized to zero, and an integer j is initialized to 1. Each array element S(i) is added with 1 that is equal to an array element S(r) and that i is less than or equal to r if the array element S(r) is equal to an array element S(r1), where r is an occurrence position of j-th atomic group of the second sequence in the first sequence. Integer j is also added with 1. The adding steps are repeated until the integer j exceeds n. A longest common atomic group number is obtained between the first and the second sequences from a value of the array element S(m).

The method further comprises preparing an array data (k) having array elements data (0), data (1)...; storing paired data (r, j) in an array element data (k) if the array element S(i) is changed in the, where k = S(r); linking the paired data (r, j) to paired data (r', j') if r' is less than r and j' is less than j, where the paired data (r', j') is one stored in an array element data (k-1); and obtaining a longest common subsequence between the first and second sequences and occurrence positions of the longest common subsequence in the first and the second sequence by tracing the link. A homology may then be evaluated between the first and the second sequences based on the longest common atomic group number and a value of one of m and n.

L27 ANSWER 4 OF 7 WPIX (C) 2003 THOMSON DERWENT

AN 2002-487852 [52] WPIX

CR 1993-308303 [39]; 2002-507172 [54]; 2002-607266 [65]; 2002-712495 [77]

DNN N2002-385480 DNC C2002-138550

TI Analyzing sequences of atomic groups by preparing memory elements corresponding to first sequence, initializing all elements to zero and obtaining longest common subsequence between chains of atomic groups.

DC B04 D16 S03 **T01**

IN **AIKAWA, S; MATSUZAWA, F; TOMIKAWA, M**

PA (FUIT) **FUJITSU LTD**

CYC 1

PI US 6370479 B1 20020409 (200252)* 61p G06F019-00 <--

ADT US 6370479 B1 US 1993-14867 19930208

PRAI **JP 1992-331703 19921211; JP 1992-21012 19920206**

IC ICM **G06F019-00**

ICS G01N033-48; G01N033-50

AB US 6370479 B UPAB: 20021204

NOVELTY - Analyzing sequences of atomic groups involves preparing memory element array with elements corresponding to a first sequence of characters, initializing all elements to zero, adding 1 to each array element that is equal to an array element with an occurrence position of

atomic group, and obtaining longest common subsequence between chains of atomic groups.

DETAILED DESCRIPTION - Analyzing sequences of atomic groups involves:

(a) inputting sequences comprising a first sequence of characters (a1 - am) and a second sequence of characters (b1 - bn) corresponding to sequences of atomic groups in first and second chains of atomic groups, respectively, where m and n are integers, into a gene information survey apparatus comprising a longest common subsequence detection unit in which b1 - bn are input from one of an amino acid sequence database and a motif database;

(b) generating an occurrence table indicating occurrence positions of a1 - am;

(c) preparing memory element array with elements S0 - Sm corresponding to a1 - am;

(d) initializing S0 - Sm to zero, and an integer j to 1;

(e) determining an occurrence position (r) of a character ar that is the same as bj by referring to the occurrence table;

(f) adding 1 to each Si where i at least r and Si = Sr-1 when Sr = Sr-1, repeating this step in decreasing order of r when there is more than one r;

(g) adding 1 to j;

(h) repeating steps (e) - (g) until j greater than n;

(i) obtaining a length of a longest common subsequence between the first and second sequences from Sm after j greater than n in step (h);

(j) analyzing the sequences of atomic groups in the first and second chains using the length of a longest common subsequence; and

(k) the sequence and results are displayed on a display device.

An INDEPENDENT CLAIM is also included for a gene information survey apparatus comprising an input device, a longest common subsequence detection unit with link array element, homology decision and search units, a motif search unit, an alignment unit and a display control unit.

USE - For analyzing sequences of atomic groups.

ADVANTAGE - The method is capable of automatically extracting and evaluating mutually coinciding or similar portions between sequences of atoms or atomic groups in molecules, e.g. protein molecules with simple processing mechanism.

DESCRIPTION OF DRAWING(S) - The figure is a block diagram showing a construction of a gene information survey apparatus.

Dwg.1/47

FS CPI EPI

FA AB; GI; DCN

MC CPI: B11-C08F1; B11-C08F3; B12-K04; D05-H09

EPI: S03-E14H; **T01-J**

TECH UPTX: 20020815

TECHNOLOGY FOCUS - INSTRUMENTATION AND TESTING - Preferred Method: The method further comprises:

(i) evaluating, in step (j), homology between the first and second sequences based on the length of the longest common subsequence and a value of one of m and n;

(ii) searching for a sequence that is homologous with the first sequence, by assigning the sequence to the second sequence and executing steps (a) - (j);

(iii) preparing a second memory element array with elements data0 - datan when n at most m, or data0 - datam when n more than m;

(iv) storing paired data (r, j) in a memory element datak if Si is changed in step (f) where k = Sr;

(v) linking paired data (r, j) stored in step (ii) with paired data (r', j') if r' less than r and j' less than j, where (r', j') is stored in datak-1;

(vi) obtaining the longest common subsequence between the first and second chains of atomic groups and occurrence positions, by tracing the link formed in step (iii).

L27 ANSWER 5 OF 7 WPIX (C) 2003 THOMSON DERWENT
 AN 1997-003764 [01] WPIX
 DNN N1997-003343
 TI 3D structure display method for analysing substance such as protein using X-ray crystal analysis appts - involves performing character display by display type corresponding to setting of display attribute of character display unit buffer.

DC **T01**
 IN **AIKAWA, S; MATSUZAWA, F; NISHINA, S**
 PA (FUIT) FUJITSU LTD
 CYC 2

PI JP 08272848 A 19961018 (199701)* 12p G06F017-50 <--
 US 6125332 A 20000926 (200051) G06F017-00 <--
 ADT JP 08272848 A JP 1995-76765 19950331; US 6125332 A US 1996-620289 19960322
 PRAI JP 1995-76765 19950331

IC ICM **G06F017-00; G06F017-50**
 ICS **G06T017-00**

AB JP 08272848 A UPAB: 19970102
 The method involves using a database (20) which stores a number of registrations of a 3D structure data of a substance. A 3D graphic display and character display of the substance is performed by referring the database. A display buffer (25) stores the 3D structure data obtained from the database and stores a setting area for the display attribute.
 A graphical display is performed by the display type corresponding to the setting of display attribute of the display buffer. A character display is performed by the display type corresponding to setting of display attribute of a character display unit buffer (30).
 ADVANTAGE - Performs display based on display state which associated graphic and character display. Provides correlation between graphic and character display. Provides wide practical usage.
 Dwg.1/14

FS EPI
 FA AB; GI
 MC EPI: **T01-J10C4B**

L27 ANSWER 6 OF 7 WPIX (C) 2003 THOMSON DERWENT
 AN 1996-043514 [05] WPIX
 DNN N1996-036531
 TI Common structure extraction unit for extracting common features of different 3D structure - has common partial extractor to extract common portion of two point assembling based on calculated accumulation distance.

DC **T01**
 IN **AIKAWA, S; MATSUZAWA, F; TOMIKAWA, M**
 PA (FUIT) FUJITSU LTD
 CYC 2

PI JP 07287717 A 19951031 (199605)* 56p G06F017-30 <--
 JP 3235763 B2 20011204 (200203) 56p G06F017-30 <--
US 6453064 B1 20020917 (200264) G06K009-00
 ADT JP 07287717 A JP 1995-10805 19950126; JP 3235763 B2 JP 1995-10805 19950126; US 6453064 B1 US 1995-390862 19950217
 FDT JP 3235763 B2 Previous Publ. JP 07287717
 PRAI JP 1994-30157 19940228

IC ICM **G06F017-30; G06K009-00**
 ICS **G06F017-50**

AB JP 07287717 A UPAB: 19960205
 The extraction unit includes a whole structure polymerization part (10) which lays two point sets (A) and whole area (B) based on partial matching information. Then, the point assembling portion which is common for both 3D structures is extracted in consideration by making a parallel rotary movement of the whole area before laying.
 A common partial length calculator computes the number of common points as pairs and assigns the value as common partial length. An accumulation distance calculator (12) computes the accumulation distance

information which indicates accumulation distance between the points that are paired. The common portion of two point assembling are extracted by an extraction unit (13) from the information computed by the accumulation distance calculation part.

ADVANTAGE - Improves accuracy and efficiency of appts.

Dwg.1/80

FS

EPI

FA

AB; GI

MC

EPI: T01-J05B3; T01-J15X

L27 ANSWER 7 OF 7 WPIX (C) 2003 THOMSON DERWENT

AN 1993-308303 [39] WPIX

CR 2002-487852 [52]; 2002-507172 [54]; 2002-607266 [65]; 2002-712495 [77]

DNN N1993-237572 DNC C1993-136720

TI Gene information testing device to evaluate similarity between aminoacid sequence and reference aminoacid - comprises unit to detect number of longest common letter between the sequences and calculation unit to find ratio of longest common letter detected.

DC B04 D16 J04 S03 S05 T01

PA (FUIT) FUJITSU LTD

CYC 1

PI JP 05219932 A 19930831 (199339)* 17p C12M001-00

ADT JP 05219932 A JP 1992-21012 19920206

PRAI JP 1992-21012 19920206

IC ICM C12M001-00

ICS G06F015-40; G06F015-42

AB JP 05219932 A UPAB: 20021204

Gene information testing device comprises a detection unit (10) to detect the number of the longest common letters between the amino acid sequence to be tested and the reference amino acid sequence each expressed by letters, and a calculation unit (11) to calculate the ratio of the number of the longest common letters detected by the detection unit (10) to the number of letters of the amino acid sequence to be tested or the reference amino acid sequence.

USE/ADVANTAGE - Used to evaluate the similarity between an amino acid sequence to be tested and a reference amino acid sequence. It is necessary for the development of medicines, etc. From the data information such as structure, function, etc. of protein can be found. In an example, where the amino acid sequence to be tested is expressed by letters 'ABCBDAB' and the reference amino acid sequence is 'BDCABA'. The detection unit detects the number of the longest common letters which is '4'; and the calculation unit calculates the ratio 57 % (= 4 - 7) to the number of letters of the amino acid sequence to be tested and 67 % (= 4 - 6) to the number of letters of the reference amino acid sequence. Thus, the similarity can be evaluated according to a simple processing mechanism.

Dwg.1a,b/1

FS

CPI EPI

FA

AB; GI

MC

CPI: B04-B04A1; B11-C08; B12-K04A; D05-H09; D05-H12; J04-B01

EPI: S03-E14H9; S05-C09; T01-J06A

=> d all abeq tech abex tot

L65 ANSWER 1 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 2003-210269 [20] WPIX

DNN N2003-167575 DNC C2003-053649

TI Identifying a site or binding region on a protein for identifying druggable regions and designing therapeutic compounds, by using mass spectrometry, nuclear magnetic resonance and X-ray diffraction analysis.

DC B04 D16 J04 K08 S05 T01

IN ARROWSMITH, C; EDWARDS, A; GREENBLATT, J; MENDLEIN, J D

PA (AFFI-N) AFFINIUM PHARM INC

CYC 100

PI WO 2003002724 A2 20030109 (200320)* EN 125p C12N000-00
 RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
 NL OA PT SD SE SL SZ TR TZ UG ZM ZW

W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
 DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
 KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
 RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM
 ZW

US 2003068650 A1 20030410 (200327) C12Q001-70

US 2003068651 A1 20030410 (200327) G01N033-53

US 2003068831 A1 20030410 (200327) G01N033-53

ADT WO 2003002724 A2 WO 2002-US7837 20020312; US 2003068650 A1 Provisional US
 2001-275216P 20010312, US 2002-97193 20020312; US 2003068651 A1
 Provisional US 2001-275216P 20010312, US 2002-97194 20020312; US
 2003068831 A1 Provisional US 2001-275216P 20010312, US 2002-97125 20020312
 PRAI US 2001-275216P 20010312; US 2002-97193 20020312; US 2002-97194
 20020312; US 2002-97125 20020312

IC ICM C12N000-00; C12Q001-70; G01N033-53

ICS G01N033-48; G01N033-50; G01N033-543; G06F019-00

AB WO2003002724 A UPAB: 20030324

NOVELTY - Identifying (M1) a site on a first protein (P1), where the site has a particular structure that is essentially not present or that is present with sufficient similarity in a second protein (P2), comprising subjecting P1 and P2 to analysis by mass spectrometry, nuclear magnetic resonance (NMR) spectroscopic analysis and X-ray diffraction analysis, and comparing the analyses of P1 with that of P2, is new.

DETAILED DESCRIPTION - Identifying (M1) a site on a first protein (P1), where the site has a particular structure that is essentially not present or that is present with sufficient similarity in a second protein (P2), such that a molecule that binds to P1 is (not) expected to bind substantially to P2, comprises subjecting purified P1 and P2 to analysis by mass spectrometry, nuclear magnetic resonance (NMR) spectroscopic analysis and X-ray diffraction analysis, and comparing the analyses of P1 with that of P2.

INDEPENDENT CLAIMS are also included for the following:

(1) determining (M2) **three dimensional** structure information of a protein, by subjecting the protein to analysis by mass spectrometry to identify the protein, subjecting the protein to structural characterization using NMR spectroscopic analysis, or X-ray diffraction analysis of a crystal of the protein;

(2) identifying (M3) a compound that binds a protein, by providing a purified protein, subjecting the protein to mass spectroscopy analysis to identify the protein, subjecting the protein to two or more of NMR spectroscopic analysis in the absence and presence of the compound, X-ray diffraction analysis in the absence and presence of the compound, and analyzing the results to identify a compound that binds to the protein;

(3) a computer readable storage medium comprising structural data which comprises the identity of P1 and P2 and **three dimensional** structure information of P1 and P2 obtained using (M1); and (4) a database comprising the identity of two or more proteins and **three-dimensional** structure information of the two or more proteins obtained using (M1).

USE - (M1) is useful for identifying a site on a first protein, where the site has particular structure that is essentially not present or that is present with sufficient similarity in a second protein, where the proteins are one of kinases, proteases, phosphatases, P450s, conjugation enzymes, ATPases, GTPases, nucleotide binding proteins, DNA processing enzymes, helicases, polymerases, RNA polymerases, DNA polymerases, G-protein coupled receptors (GPCRs), intracellular receptors, metabolic enzymes, nuclear receptors, channels, phosphodiesterases, Ca binding proteins, bacterial proteins, non-membrane bacterial proteins, human proteins that bind viral proteins, viral proteins, or non-membrane viral

proteins. (M1) is useful for identifying a compound, preferably a polypeptide, nucleic acid or a small molecule, that binds specifically to P1 relative to P2 or that binds to P1 and P2, where P2 is a mutant of P1, both are orthologs, and are from different microbial or mammalian species. The compound is isolated from naturally occurring source, or is a member of library of compounds. (M2) is useful for determining **three-dimensional** structure information of a protein, preferably of bacterial origin. (M3) is useful for identifying a compound that binds a protein from mammalian or microbial species (all claimed).

Dwg.0/0

FS CPI EPI

FA AB; DCN

MC CPI: B04-L01; B04-N04; B11-C07B2; B11-C07B5; B11-C08A; B11-C09; B12-K04E; D05-H09; J04-B01; K08-X; K09-B

EPI: S05-D02B; T01-J06A1; T01-S03

TECH UPTX: 20030324

TECHNOLOGY FOCUS - BIOTECHNOLOGY - Preferred Method: P1 and P2 are structurally related or unrelated proteins, have similar biological activity, homologs of each other and have 80% amino acid sequence identity. P1 and P2 are in the same biosynthetic pathway. The atomic coordinates for the two or more proteins have a **root mean square** deviation of not more than 1.5Angstrom for all backbone atoms shared in common in the site, and for all side chain atoms and Calpha atoms shared in common in the site. (M1) further comprises repeating all the steps on a **third** protein and including the protein in the comparison. The method is repeated on at least 10% of the polypeptides in a defined proteome and including the polypeptides in the comparison. The defined proteome comprises non-membrane proteins, membrane proteins, proteins in an organelle, or proteins in a pathway. A compound that binds to the site on P1 is identified using structure guided drug design, which comprises supplying a computer modeling application with a **set** of structure coordinates and structural information obtained for P1 and P2, and supplying the computer modeling application with a **set** of structure coordinates for a chemical entity. The potential binding interactions between the chemical entity and the site of P1 is evaluated, and the chemical entity is structurally modified to yield a **set** of structure coordinates for a modified chemical entity, and the chemical entity is expected to bind to P1 is determined. The structure guided drug design further comprises performing a fitting operation between the chemical and the site of P1, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the site of P1. The method further comprises identifying a compound that is expected to bind to the site on P1 and determining the ability of the compound to bind to P1 and P2 using an activity assay, where a change in the activity of one of the proteins in the presence of the compound indicates that the compound modulates the activity of the protein. The mass spectrometry analysis identifies the primary sequence of the protein, the type and location of post translational modifications of the protein, or identifies regions of the protein which interact with another molecule. The NMR spectroscopic analysis involves one **dimensional** NMR, two **dimensional** NMR or 15N/1H correlation spectroscopy. Several of the experimental procedures for one or more of the analyses are automated. Either of the crystallized P1 or P2 diffracts X-rays to a resolution of 3.5Angstrom or better. (M1) further comprises subjecting P1 and P2 to the proteolytic digestion prior to the analysis by mass spectrometry. The NMR spectroscopic analysis is used to determine information about the **three dimensional** structure, the conformational state, the aggregation level or the state of unfolding of the protein. The X-ray diffraction is used to determine the **three dimensional** structure of P1 and P2. P1 and P2 comprise one or more isotopic labels such as 40K, 14C, 3H, 35S, 32P, 99mTc, 201Tl, 67Ga, 111In, 123I, 131I,

90Y, 153Sm, 186Re, 188Re, 165Dy, 166Ho, 1H, 2H, 3H, 31P, 23Na, 14N, 15N, 13C and 19F, or a heavy atom label such as cobalt, selenium, krypton, bromine, strontium, molybdenum, ruthenium, gadolinium, terbium, dysprosium, holmium, erbium, ytterbium, tantalum, tungsten, rhenium, osmium, iridium, platinum, gold, mercury, thallium, lead, thorium and uranium. P1 and P2 comprise at least one seleno-methionine, and are at least 70% soluble as measured by light scattering, and are fused to a heterologous polypeptide.

ABEX

UPTX: 20030324

WIDER DISCLOSURE - Also disclosed are:

- (a) kits for carrying out the above methods;
- (b) making a compound that binds to a site of interest on a protein or complex;
- (c) generating **sets** of combinatorial mutants of polypeptides;
- and

(d) a computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or molecular complex.

EXAMPLE - Analytical samples containing peptides produced by limited or complete proteolytic digestion were subjected to matrix assisted laser desorption/ionization time of flight (MALDI-TOF) mass spectrometry. Analysis of the peptides in the mass spectrometer was conducted using both delayed extraction mode and an ion reflector to ensure high resolution of the peptides. Internally-calibrated peptide masses were searched against databases using a correlative mass matching algorithm. Identified proteins were stored automatically in a relational database with software linked to sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) images and ligand sequences. Tryptic peptides were analyzed. Samples containing peptides produced by limited or complete proteolytic digestion were analyzed with an ion trap instrument. All resulting mass spectra were submitted to a database search algorithm for protein identification. A correlative mass algorithm was utilized along with a statistical verification of each match to identify a protein's identification. Nuclear screening experiments were performed on a Varian Unity 500 spectrometer. The data was then processed on a Sun Ultra 5 computer with nuclear magnetic resonance (NMR)pipe software. The proteins were then analyzed by X-ray crystallography.

L65 ANSWER 2 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 2003-112007 [10] WPIX

DNN N2003-089147 DNC C2003-028697

TI Identifying a search model to use in molecular replacement for determining a structure of a target biomolecule from crystal data comprises employing computer executable logic.

DC B04 D16 T01

IN ABOLA, E; DAVID, P R; DELFT, F V; MCREE, D; RAMMELKAMP, J; VON DELFT, F
PA (ABOL-I) ABOLA E; (DAVI-I) DAVID P R; (DELF-I) DELFT F V; (MCRE-I) MCREE
D; (RAMM-I) RAMMELKAMP J; (SYRR-N) SYRRX INC

CYC 100

PI WO 2002091287 A2 20021114 (200310)* EN 58p G06K009-00

RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
NL OA PT SD SE SL SZ TR TZ UG ZM ZW

W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM
ZW

US 2002183861 A1 20021205 (200310) G05B015-00

ADT WO 2002091287 A2 WO 2002-US13988 20020503; US 2002183861 A1 US 2001-848866
20010504

PRAI US 2001-848866 20010504

IC ICM G05B015-00; G06K009-00

AB WO 200291287 A UPAB: 20030211

NOVELTY - Identifying a search model to use in molecular replacement for determining a structure of a target biomolecule from crystal data comprises employing computer executable logic.

DETAILED DESCRIPTION - Identifying a search model to use in molecular replacement for determining a structure of a target biomolecule from crystal data comprises:

(a) employing computer executable logic to perform multiple molecular replacement searches on crystal data of the target biomolecule, where a group of different biomolecule structures are used as search models for the multiple molecular replacement searches; and

(b) employing computer executable logic to compare solutions from the multiple molecular replacement searches, where the comparison produces data from which biomolecule structures in the group can be identified as having superior structural identity with the target biomolecule as compared to the other biomolecule structures in the group.

An INDEPENDENT CLAIM is also included for a computer readable medium, useful in association with a computer that includes a processor and a memory, comprising:

(a) logic for performing multiple molecular replacement searches on crystal data or diffraction data of a target biomolecule where a group of different biomolecule structures are used as search models for the multiple molecular replacement searches; and

(b) logic for comparing solutions from the multiple molecular replacement searches.

USE - The method is useful for identifying a search model in molecular replacement for determining a structure of a target biomolecule from crystal data (claimed).

Dwg.0/3

FS CPI EPI

FA AB; DCN

MC CPI: B04-E01; B04-N04; B11-C08F1; B11-C08F3; B11-C08G; B11-C09; B12-K04E; D05-H09; D05-H12

EPI: T01-E01C; T01-J03; T01-J04B1; T01-J05B3; T01-J15H; T01-S03

TECH UPTX: 20030211

TECHNOLOGY FOCUS - BIOTECHNOLOGY - Preferred Method: Identifying a search model for use in molecular replacement for determining a structure of a target biomolecule from crystal data further comprises employing computer executable logic to select the group of different biomolecule structures used to perform the multiple replacement searches. The biomolecule is a protein, DNA, RNA or a complex comprising a protein, DNA or RNA. The crystal data is X-ray diffraction data, neutron diffraction crystal data, magnetic crystal data, nuclear magnetic resonance crystal data or mass spectrometry crystal data. Molecular replacement is performed using a program comprising AmoRe, BRUTE, COMO (Combined molecular replacement), CNS (Crystallography and NMR System), TNT, GLRF (General locked rotation function program), TRANSF (Translation function program), TF (translation function program), ENVELOPE (Real Space Molecular averaging and Envelope Finding program), FFSYNTH (P1 FFT synthesis (reciprocal to direct space) program), FFTINV (Fourier inversion direct to reciprocal space) program) or FFTEXP (Reflection data expanding program), preferably EPMR (a program that finds crystallographic molecular replacement solutions using an evolutionary search algorithm), or a molecular replacement program comprising an evolutionary algorithm for searching six-dimensional space.

Comparing molecular replacement solutions comprises:

(a) comparing figures of merit calculated for the molecular replacement solutions;

(b) performing a statistical analysis on figures of merit calculated for the molecular replacement solutions;

(c) determining which of the biomolecule structures in the group produced a molecular replacement solution whose figure of merit is at least two, **three**, five or ten standard deviations better than the average figure of merit for molecular replacement solutions for the biomolecule

structures in the group;

(d) comparing **root mean square** errors for each molecular replacement solution of a probability-weighted average over all possible phase choices;

(e) establishing a background correlation level between the biomolecule structures in the group and the target biomolecule based on the molecular replacement solutions and determining which of the biomolecule structures in the group produced a molecular replacement solution that exceeds the background correlation level by at least two, **three**, five or ten standard deviations.

The group of different biomolecule structures on which molecular replacement searches are performed comprises:

(a) at least 3 different biomolecule structures, at least one biomolecule structure that has less than 70% sequence identity with the target biomolecule or at least two different biomolecule structures that are structurally dissimilar to each other or that have less than 70% sequence identity with each other;

(b) at least 0.1% of the protein structures stored in the Protein Data Bank; or

(c) at least one predicted structure for a biomolecule; or

(d) at least one structure where at least a portion of the native structure has been removed or which comprises a combination of two or more structure fragments. The data produced from the comparison identifies which biomolecule structures produced molecular replacement solutions that are at least among the top 35% of molecular replacement solutions produced by the group, or that are at least 2, 3, 5 or ten standard deviations better than the molecular replacement solutions produced by the group.

Selection of the group of biomolecule structures is:

(a) based, at least in part, on sequence identity between the biomolecule structure and the target biomolecule; or

(b) at least partially random or completely random, or is iterative.

Selection of the members of the group of biomolecule structures is performed until a biomolecule structure is selected whose molecular replacement solution is at least 2, 3, 5 or ten standard deviations better than the molecular replacement solution for the biomolecule structures in the group.

ABEX

UPTX: 20030211

EXAMPLE - No suitable example given.

L65 ANSWER 3 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 2002-627346 [67] WPIX

DNN N2002-496115 DNC C2002-176918

TI Identifying a pharmacocluster, by determining bound conformations of a ligand bound to different polypeptides, and clustering two or more bound conformations of the ligand having substantially same bound conformation.

DC B04 D16 S03 T01

IN HANSEN, M; SEM, D S

PA (HANS-I) HANSEN M; (SEMD-I) SEM D S; (TRIA-N) TRIAD THERAPEUTICS INC

CYC 100

PI WO 2002056236 A2 20020718 (200267)* EN 225p G06F019-00

RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
NL OA PT SD SE SL SZ TR TZ UG ZM ZW

W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM
ZW

US 2002133296 A1 20020919 (200269) G06F019-00

ADT WO 2002056236 A2 WO 2001-US50608 20011219; US 2002133296 A1 US 2000-747174
20001222

PRAI US 2000-747174 20001222

IC ICM G06F019-00

ICS G01N033-48; G01N033-50; G01N033-68

AB WO 200256236 A UPAB: 20021018

NOVELTY - Identifying (M1) a pharmacocluster, comprising determining bound conformations of a ligands bound to different polypeptides, and clustering two or more bound conformations of the ligand having substantially the same bound conformation, therefore identifying a pharmacocluster, is new.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:

(1) identifying (M2) a member of a pharmacocluster, comprises determining a bound conformation of a ligand bound to a polypeptide, and determining a pharmacocluster having substantially the same bound conformation as the bound conformation, therefore identifying the bound conformation of the ligand as a member of the pharmacocluster;

(2) identifying (M3) a conformation-dependent property of a ligand, comprises determining bound conformations of a ligand bound to a different polypeptide, identifying two or more bound conformations of the ligand having substantially the same bound conformation, and identifying a conformation-dependent property of the bound conformations of the ligand having substantially the same bound conformations (the conformation-dependent property is correlated with the bound conformation of the ligand);

(3) identifying (M4) polypeptide pharmacofamilies, comprises determining bound conformations of a ligand bound to different polypeptides of a polypeptide family, and identifying 2 or more bound conformations of the ligand having substantially different bound conformations, therefore identifying at least two polypeptide pharmacofamilies exhibiting binding specifically for the two or more substantially different bound conformations of the ligand;

(4) identifying (M5) a member of a polypeptide pharmacofamily, comprises determining conformation-dependent property of a ligand bound to a polypeptide, and determining a pharmacocluster having substantially the same conformation-dependent property as the conformation-dependent property determined for the bound ligand (a polypeptide pharmacofamily binds the ligand in a conformation of the pharmacocluster), therefore identifying the polypeptide as a member of the polypeptide pharmacofamily;

(5) modeling (M6) the **three dimensional** structure of a polypeptide, comprises M5 followed by modeling the **three dimensional** structure of a polypeptide according to a structural model of the second member of the polypeptide pharmacofamily;

(6) constructing (M7) a ligand conformer model, comprises determining an average structure of the bound conformations of a ligand in a pharmacocluster;

(7) constructing (M8) a pharmacophore model, by constructing a model that contains one or more selected conformation-dependent properties of one or more pharmacoclusters;

(8) identifying (M9) a binding compound for one or more members of a polypeptide pharmacofamily, by identifying a compound having a selected conformation-dependent property of a pharmacocluster;

(9) a pharmacocluster (I) is selected from pharmacocluster 1-8;

(10) a polypeptide pharmacofamily (II) comprising polypeptides that bind to substantially the same bound conformation of a nicotinamide adenine dinucleotide-related molecule selected from pharmacofamily 1-8 or that bind to nicotinamide adenine dinucleotide-related molecule having a bound conformation selected from pharmacocluster 1-8;

(11) a ligand conformer model (III), comprising a ligand conformer model, selected from a conformer model 1-8 having coordinates given in the specification;

(12) a moiety (IV) comprising coordinates, selected from O2A, OP3, A15, A22, N7A, C6N, or C8A given in the specification; and

(13) a pharmacophore model (V) comprising a pharmacophore model selected from pharmacophore model 1-8 having coordinates given in the specification.

USE - M1 is useful for identifying a pharmacocluster (claimed). (V) is useful in querying a database of polypeptide structures to find other

members of the polypeptide pharmacofamily and also to design a binding compound that is specific for polypeptides of one or more pharmacofamilies.

Dwg.0/7

FS CPI EPI

FA AB; DCN

MC CPI: B04-C01; B04-C02; B04-G01; B04-L01; B04-N01; B04-N04; B11-C08E;

B11-C08F; B11-C08G; B11-C10; B12-K04E; D05-H09

EPI: S03-E14H5; T01-J05B4P; T01-J06A

TECH UPTX: 20021018

TECHNOLOGY FOCUS - BIOTECHNOLOGY - Preferred Method: In M1, substantially the same bound conformation comprises a **root mean square** deviation of less than 1.1 Angstrom. In M1, M2, M3, M4 and M5, the ligand is selected from adenosine triphosphate, adenosine diphosphate, adenosine monophosphate thiamine (vitamin B1), riboflavin (vitamin B2), pyridoximine (vitamin B6), cobalamin (vitamin B12), pyrophosphate, flavin adenine dinucleotide (FAD), flavin mononucleotide (FMN), pyridoxal phosphate, coenzyme A, ascorbate (vitamin C), niacin, biotin, heme, porphyrin, folate, tetrahydrofolate, guanosine triphosphate, cytidine triphosphate, thymidine triphosphate, uridine triphosphate, retinol (vitamin A), calciferol (vitamin D2), ubiquinone, ubiquitin, alpha-tocopherol (vitamin E), farnesyl, geranylgeranyl, pterin, pteridine or S-adenosyl methionine (SAM).

The ligand comprises a nicotinamide adenine dinucleotide-related molecule, which is selected from oxidized nicotinamide adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, or its mimetic. In M3, the conformation-dependent property comprises a spectroscopic signal or nuclear magnetic resonance (NMR) signal. The NMR signal is selected from chemical shift, J coupling, dipolar coupling, cross-correlation, nuclear spin relaxation, transferred nuclear overhauser effect, or its combinations. In M4, the polypeptide pharmacofamily is selected from pharmacofamily 1-8. In M5, the ligand is a adenosine phosphate-related molecule selected from adenosine triphosphate, adenosine diphosphate, adenosine monophosphate or its mimetic.

ABEX UPTX: 20021018

EXAMPLE - Polypeptide pharmacofamilies based on bound conformation of NAD(P)(H) ligands was identified. The oxidoreductases form a family of polypeptides that bind NAD(H) and NADP(H). In order to identify pharmacofamilies within the family of oxidoreductases, bound conformations of NAD(P)(H) were determined by searching the protein databank. Bound conformations from 156 structures were clustered into separate pharmacoclusters, and pharmacofamilies were identified according to binding to bound conformations of NAD(P)(H) in separate pharmacoclusters. Structure files containing polypeptides with bound NAD(P)(H) were identified from the protein databank. All clusters were visually inspected using Insight 98 for outliers that demonstrated poor overlay with the rest of the pharmacocluster as a whole. These outliers were compared against each other and existing pharmacoclusters to find other possible matches. Those that did not fit any family were removed. Comparison between bound conformations was made based on the RMSD equations supplied in COMPARE. 8 pharmacoclusters were identified. Visual inspection of the clusters demonstrated that members within a cluster were substantially overlapped. Comparison between clusters demonstrated substantial differences. The dihedral angles for various bonds in the bound conformations of the NADP(H) ligand could be used to distinguish the pharmacoclusters. Although many dihedral angles were similar between 2 or more pharmacoclusters, each pharmacocluster could be distinguished from the others by comparison of the full **set** of dihedral angles. For e.g., pharmacoclusters 2 and 3 can be distinguished by comparison between the dihedral angles at O4'A-C4'A-C5'A-O5'A which were 154degrees and -131degrees, respectively and by comparison between the dihedral angles at C5'A-O5'A-PA-O3 which were 105degrees and 57degrees, respectively.

A quantitative analysis of the results of clustering bound conformations of NAD(P)(H) was determined and were fully given in the specification. Average coordinates were determined from the pharmacocluster **subsets**. The RMSD values for each member were calculated as comparisons to an average structure for the **subsets**. For each pharmacocluster a **subset** of the possible ligands that belong to each cluster were identified. Each **subset** was chosen to maximize the diversity of the family and to minimize over-representation of ligand conformations from enzymes that exist multiply in the PDB database. The goal of the **subset** selection was to fully represent characteristics from oxidoreductases belonging to a range of species and catalyzing a range of different reactions. The 3-dimensional coordinates for each atom in each ligand were used to calculate an average position and a standard deviation for the pharmacofamily.

The results demonstrated that bound conformations of a ligand could be grouped into pharmacoclusters by a structure comparison. These results also demonstrated the distinguishing pharmacoclusters and members within pharmacoclusters.

L65 ANSWER 4 OF 18 WPIX (C) 2003 THOMSON DERWENT
 AN 2002-590545 [63] WPIX
 CR 2001-597203 [67]
 DNN N2002-468655 DNC C2002-167008
 TI Producing model of desired region involves collecting **set** of data **points** for region, dividing data **set**, interpolating data **points** in model, comparing and varying model data **points** to data **sets**.
 DC B04 D16 H01 J04 T01
 IN ORTOLEVA, P J
 PA (ORTO-I) ORTOLEVA P J; (USGO) US GOVERNMENT
 CYC 99
 PI WO 2002047011 A1 20020613 (200263)* EN 112p G06G007-48
 RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
 NL OA PT SD SE SL SZ TR TZ UG ZM ZW
 W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
 DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
 KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
 RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZM ZW
 US 2002120429 A1 20020829 (200264) G06F017-10
 AU 2002039619 A 20020618 (200266) G06G007-48
 ADT WO 2002047011 A1 WO 2001-US48589 20011207; US 2002120429 A1 Provisional US
 2000-254433P 20001208, CIP of US 2001-818752 20010327, US 2001-17829
 20011207; AU 2002039619 A AU 2002-39619 20011207
 FDT AU 2002039619 A Based on WO 200247011
 PRAI US 2001-818752 20010327; US 2000-254433P 20001208; US 2001-17829
 20011207
 IC ICM G06F017-10; G06G007-48
 AB WO 200247011 A UPAB: 20021031
 NOVELTY - Producing (M1) a model of desired region involves collecting a first **set** of data **points** (DP) pertaining to the desired region, dividing first data **set** into second and third data **sets**, interpolating DP in the model using a **subset** of DPs from second data **set**, comparing model DPs to DPs of third data **set**, varying model DP corresponding to DP in the second data **set** and repeating the interpolating and comparing.
 DETAILED DESCRIPTION - Producing (M1) a model of a region of interest, involves collecting a first **set** of data **points** pertaining to the region of interest, dividing the first data **set** into a second data **set** and a third data **set**, populating a model with data **points** from the second data **set**, interpolating a data **point** in the model using a **subset** of data **points** from the second data **set**

, comparing a **subset** of data **points** in the model to a **subset** of data **points** in the third data **set**, and if comparing yields a discrepancy larger than an error limit, then varying a data **point** in the model corresponding to a data **point** in the second data **set** and repeating the interpolating and comparing.

INDEPENDENT CLAIMS are also included for:

(1) extending (M2) a model of a region of interest along a coordinate, which involves applying an equation to evolve the model a distance along the coordinate and maximizing a probable state of the evolved model;

(2) estimating (M3) a probability of a model of a region of interest, which involves collecting a **set** of data **points** pertaining to the region of interest, comparing a **subset** of data **points** in the model to a **subset** of data **points** in the collected data **set** to yield a discrepancy, and calculating a probability functional that maximizes an entropy, the calculating subject to normalizing the probability functional and subject to a constraint based on a **subset** of data **points** in the collected data **set**;

(3) producing (M4) a model of fracture locations and fracture characteristics in a geologic basin or producing a model of biological cell, which involves collecting a first **set** of data **points** pertaining to the geologic basin or biological cell, dividing the first data **set** into a second data **set** and a third data **set**, populating a model with data **points** from the second data **set**, processing a **subset** of data **points** in the model by applying equations to simulate rock rheology by integrating continuous deformation with fracture, fault, gouge, and pressure solutions, or simulate reactions, the equation is of types in the **set** which is a chemical kinetic, proteomic, genomic, glycolysis, citric acid cycle, amino acid synthesis, nucleotide synthesis or membrane transport, processing a **subset** of data **points** in the model by applying equations to simulate mechanical processes to coevolve deformation with multi-phase flow, petroleum generation, mineral reactions, and heat transfer, comparing a **subset** of data **points** in the model to a **subset** of data **points** in the third data **set**, and if comparing yields a discrepancy larger than an error limit, then varying a data **point** in the model corresponding to a data **point** in the second data **set** and repeating the processing and comparing; and

(4) a computer readable medium (I) having instructions for performing M1, M2, M3 and M4.

USE - Useful for producing a model of desired region (claimed).

ADVANTAGE - M1 greatly reduces the sensitivity coefficient calculations, increasing with the number of grid nodes on which the most probable reservoir state is obtained.

DESCRIPTION OF DRAWING(S) - The figure shows a schematic flow chart of the simulation-enhanced fracture detection data modeling/integration approach to geologic basins.

Dwg.1/57

FS CPI EPI

FA AB; GI

MC CPI: B11-C08E2; B11-C08H; B12-K04E; D05-H09; H01-A; J04-B01

EPI: T01-J03; T01-S03

TECH UPTX: 20021001

TECHNOLOGY FOCUS - BIOTECHNOLOGY - Preferred Method: In M1, collecting step involves collecting data **points** of more than one type.

Dividing produces data **points** common to the second and third data **sets**. Interpolating involves applying multi-dimensional, finite-element methods to a **subset** of data **points** in the model or applying an equation to a **subset** of data **points** in the model, where the equation is of a type in

the **set** thermodynamic, chemical, or genomic. Interpolating is based, at least in part, on a spacing among or on measure of constraint of a **subset** of data **points** in the model. Comparing yields a discrepancy based, at least in part, on a sum of squares of differences between a **subset** of data **points** in the model and a **subset** of data **points** in the **third** data **set**. Varying a data **point** involves varying an item in the **set**, which is a value of the data **point**, or a position of the data **point** in the model. Varying involves varying multiple data **points** in the model corresponding to data **points** in the second data **set**. Collecting involves associating measures of constraint with data **points** in the second data **set** and where varying involves choosing a data **point** in the model to vary, the chosen data **point**'s measure of constraint is less than that of another data **point** in the model. Measure of constraint is associated with a probable error range and where a larger error range yields a lower constraint. M1 further involves estimating a probability of the model resulting from the varying, where the varying involves choosing an amount by which to vary a data **point**, the data **point** and the amount to vary the data **point** chosen, at least in part, in order to maximize an estimated probability of the model. Estimating a probability is subjected to a constraint based on a **subset** of data **points** in the **third** data **set**. Estimating a probability involves calculating a probability functional that maximizes an entropy, the calculating subject to normalizing the probability functional and subjected to a constraint based on a **subset** of data **points** in the **third** data **set**. Entropy is defined to comprise a negative of a functional integral over possible states of the model of the probability functional multiplied by a natural log of the probability functional. Normalizing the probability functional involves setting a functional integral over possible states of the model of the probability functional to one. The calculating is subjected to a constraint based on a **subset** of data **points** in the **third** data **set** when a functional integral over possible states of the model of the discrepancy multiplied by the probability functional is equal to an ensemble error average. Maximizing an estimated probability of the model involves determining where a functional derivative of the probability functional with respect to the model becomes zero. In M2, maximizing a probable state involves collecting a **set** of data **points** pertaining to the region of interest, comparing a **subset** of data **points** in the model to a **subset** of data **points** in the collected data **set**, and if comparing yields a discrepancy larger than an error limit, then varying a data **point** in the model and repeating the comparing. In M4, collecting a first **set** of data **points** involves collecting data in the **set**: well log data, surface data, core data, seismic data or microscopy, genomics, proteomics, multidimensional spectroscopy, X-ray crystallography, thermodynamics, biochemical kinetics, or bioelectrics.

L65 ANSWER 5 OF 18 WPIX (C) 2003 THOMSON DERWENT
 AN 2002-480088 [51] WPIX
 DNN N2002-379134 DNC C2002-136649
 TI Homology modeling-based method for constructing a **three-dimensional** structure of a protein, comprises aligning with a structurally-known referential protein and using alignment data, applicable in e.g. the design of drugs.
 DC B04 C07 D16 T01
 IN IWADATE, M; UMEYAMA, H
 PA (MITU) MITSUBISHI CHEM CORP; (UMEY-I) UMEYAMA H
 CYC 99
 PI WO 2002044954 A1 20020606 (200251)* JA 111p G06F017-50

RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
 NL OA PT SD SE SL SZ TR TZ UG ZM ZW
 W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
 DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
 KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
 RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZM ZW

AU 2002022563 A 20020611 (200264) G06F017-50

ADT WO 2002044954 A1 WO 2001-JP10438 20011129; AU 2002022563 A AU 2002-22563
 20011129

FDT AU 2002022563 A Based on WO 200244954

PRAI JP 2000-368415 20001204; JP 2000-367007 20001201

IC ICM G06F017-50

AB WO 200244954 A UPAB: 20021031

NOVELTY - Constructing the **three-dimensional** (3D) structure of a protein comprises aligning an arbitrary target protein with a referential protein having a known 3D structure then constructing the 3D structure of the target protein based on the selected referential protein and alignment data.

DETAILED DESCRIPTION - Constructing the **three-dimensional** (3D) structure of a protein comprises aligning an arbitrary target protein with a referential protein having a known 3D structure then constructing the 3D structure of the target protein based on the selected referential protein and alignment data, during which the alignment is corrected with use of the 3D structure information obtained from coordinates of the referential protein before construction of the 3D structure by basing on the corrected alignment.

INDEPENDENT CLAIMS are also included for the following:

(1) a similar method in which the alignment is carried out by using high homology for alignment and 2 types of software for profile alignment, and the results are then based for selection of the referential protein and alignment;

(2) another similar method where lengths of inserted partial sequences are obtained for the initial construction of alignment, after which:

(a) the alignment is conducted with removal of some lengths from the inserted partial sequences of the target protein to match the referential protein;

(b) a C alpha atom coordinate of the target protein is constructed after tidying up;

(c) further trimming of amino acid sequences from terminals of the resultant target protein is performed to refine the alignment;

(d) after re-alignment with trimming of the C alpha atom coordinate of the original target protein is subsequently produced; and

(e) the inserted partial sequences are removed and the residual groups at the corresponding parts are cleaved or replaced to form the required C alpha atom coordinate in the original target protein through repeated operations;

(3) separating domains in a protein by performing a homology search on a sequence with 3D structure but unknown domain break-points against a sequence with 3D structure and known domain break-points, after which consensus of the homologous sequence of each of the obtained domains is based for determining the domain break-points;

(4) a database for the domain unit-separated 3D structures thus constructed;

(5) a referential protein search via an amino-acid sequence database comprising carrying out a homology search of any target protein with use of the amino-acid sequence database, a further homology search on a 3D structure database basing on the obtained amino acid sequence to select a required protein sequence from the database for reference in aligning with that of the target protein;

(6) atom coordinates for specified 3D structures of

proteins thus obtained;

(7) computer-readable recording media for storing the atom coordinates;

(8) a database containing the atom coordinates; and

(9) a molecular design method for drugs based on 3D structures of proteins constructed with use of the atom coordinates, or the recording media or atom coordinates in the database, for interaction with the 3D structures of drug candidate molecules, so that targeted drug molecules can be identified, searched, evaluated or designed.

USE - The method is for constructing **three-dimensional** structure of a protein, which is applicable in design of drugs (claimed) and agrochemicals.

ADVANTAGE - With this accurate and efficient construction method, the obtained alignment can be corrected to eliminate specific manner in selection and sequence redundancy.

Dwg.0/43

FS CPI EPI

FA AB; DCN

MC CPI: B04-N04; B11-B; B11-C08F3; B11-C09; B12-K04; B12-K04E; C04-N04; C11-B; C11-C08F3; C11-C09; C12-K04; C12-K04E; D05-H; D05-H09; D05-H18
EPI: T01-J15

TECH UPTX: 20020812

TECHNOLOGY FOCUS - INSTRUMENTATION AND TESTING - Preferred Methods: In the construction methods, when profile alignment is applied in the alignment, the profile data are also considered for alignment correction. The 3D structure data are secondary structure data, hydrophobic core values and hydrophobic core distances. To construct the 3D structure, the Calpha atom in an amino acid related coordinate is obtained from a 3D structure of the referential protein, so that the target correlation coefficient can be minimized for optimization of the Calpha atom coordinate then the rest of the main and side-chain atom coordinates are similarly optimized to provide an optimum structure. When selecting referential protein and alignment, a high homology software is used for re-alignment between plural alignments after calculation by 2 types of software and compared, and in the case of such homology being high, the e value in the target protein that is higher than the referential protein and alignment is eliminated. Such software for high homology-used alignment is FASTA, while the profile alignment-used software is PSI-BLAST (Basic Local Alignment Search tool). When several alignments are obtained, candidates will be selected by the software each of which is considered by basing on the referential protein and alignment data for calculation of Calpha atom coordinate of the target protein, and fitting of the fellow Calpha atom coordinates in the 3D structure is conducted. In the case of the **root-mean-square** distance (RMSD) of various coordinates is judged as below a certain value, the high e values of the referential protein and alignment are eliminated from the target protein, and then the referential protein and alignment is selected. Such RMSD is particularly 3 Angstrom. After the manipulation, the 3D structure can be constructed by obtaining the Calpha atom coordinates in an amino acid from a 3D structure of the referential protein then the other atom coordinates in the main and side-chains in the target protein. Separated domain units are selected with use of a 3D structure database in construction of the 3D structure of the target protein by basing on the referential protein. In the domain-separating method when a homologous sequence in each of the thus obtained domain has an identifier, the identifier of the determined domain is judged by basing on the consensus of the identifier. If several sequences of the target protein are homologous to sequences in the amino-acid sequence database, high homology alignment is applied to eliminate sequence redundancy. The elimination of sequence redundancy is particularly conducted on variable judgement basis in a stepwise manner. Up to 10 sequence redundancies can be eliminated

from the detected sequences of the amino-acid sequence database. When plural alignments are obtained, the unmatched parts are identified from the matched parts between these alignments by basing on their consensuses to give a single alignment. Having detected homology with sequences in the 3D structure database, 3D structure of the target protein is constructed with selection of sequences by basing on the referential protein.

ABEX UPTX: 20020812

EXAMPLE - After a PSI-BLAST (Basic Local Alignment Search Tool (BLAST) search in Escherichia coli genome 3D structure database protein DataBank (PDB), the 3D structure of the open reading frame (ORF), clpP, was constructed by alignment correction, with e value being not more than 0.001.

L65 ANSWER 6 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 2002-433750 [46] WPIX

CR 1998-557712 [47]

DNN N2002-341308

TI Microscopy imaging method involves removing spatial pattern and obtaining in-focus image by calculating **square root** of sum of **squares** of differences between recorded images in each pair of images.

DC S02 S03

IN JUSKAITIS, R; NEIL, M A A; WILSON, T

PA (ISIS-N) ISIS INNOVATION LTD

CYC 1

PI US 6376818 B1 20020423 (200246)* 11p G01B011-06

ADT US 6376818 B1 CIP of WO 1998-GB988 19980403, US 1999-410614 19991001

PRAI US 1999-410614 19991001; WO 1998-GB988 19980403

IC ICM G01B011-06

AB US 6376818 B UPAB: 20020722

NOVELTY - The method involves removing the spatial pattern and obtaining an in-focus image by calculating the **square root** of the sum of the **squares** of the differences between the recorded images in each pair of images. The recorded images of the specimen are grouped into pairs of images such that the pattern spatial phase is different for each recorded image.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:

(a) a microscopy imaging apparatus;

(b) and a method of adapting a microscope to produce optically sectioned images of a specimen.

USE - Used for generating the in-focus **three-dimensional** images of volume structures.

ADVANTAGE - Achieves optical sectioning of the images without the need for precise alignment or matching of the detector and the pattern components. Enables producing optically sectioned images from a microscope in real time since image data processing is simplified. Enables readily converting microscopes or ubiquitous piece of laboratory equipment to provide optical sectioned images.

DESCRIPTION OF DRAWING(S) - The figure shows the schematic block diagram of the microscopy imaging apparatus.

Dwg.1/4

FS EPI

FA AB; GI

MC EPI: S02-J04B1; S02-K01; S03-E04R

L65 ANSWER 7 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 2002-362627 [39] WPIX

CR 2001-596685 [67]; 2002-113884 [15]; 2002-279946 [32]; 2003-287703 [28]

DNN N2002-283383

TI Distance measurement in **three-dimensional** image acquisition systems, involves combining output signals of sensor, acquired

at higher repetition rate so that random noise in measurement is reduced.

DC S02 T01 T04 U21
IN BAMJI, C; RAFII, A; SZE, C; TORUNOGLU, I
PA (CANE-N) CANESTA INC
CYC 96
PI WO 2002029711 A2 20020411 (200239)* EN 95p G06K009-00
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
NL OA PT SD SE SL SZ TR TZ UG ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PH PL PT RO
RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG UZ VN YU ZA ZW
AU 2002011439 A 20020415 (200254) G06K009-00
ADT WO 2002029711 A2 WO 2001-US31163 20011003; AU 2002011439 A AU 2002-11439
20011003
FDT AU 2002011439 A Based on WO 200229711
PRAI US 2000-684368 20001005
IC ICM G06K009-00
AB WO 200229711 A UPAB: 20030501
NOVELTY - The output signals from a **three-dimensional**
sensor (20) obtained at higher repetition rate are combined to obtain the
average output signal such that the random noise in a **three-**
dimensional sensor system (10) is reduced in proportion to the
square root of number of the averaged output signals.
DETAILED DESCRIPTION - INDEPENDENT CLAIMS are included for the
following:
(a) Z-values encoding method;
(b) Computer readable storage medium storing distance measurement
program; and
(c) Computer readable medium storing Z-values encoding program.
USE - In **three-dimensional** image acquisition
system for measuring time-of-fly and distance of users fingers on virtual
input device such as keyboard of computer, laptop, PDA, wireless
telephone, pen-based computer, virtual data input system, hands free
interactive computing system, game machine, electronic cash register,
interactive television, and other electrical appliances used in security
and identification applications.
ADVANTAGE - Improves distance measurement accuracy by reducing noise
in the system.
DESCRIPTION OF DRAWING(S) - The figures show the **three-**
dimensional sensor systems.
Three-dimensional sensor system 10
Three-dimensional sensor 20
1A, 1B/17
FS EPI
FA AB; GI
MC EPI: S02-B12; T01-C02A; T01-C08B; T01-S03; T04-F01A5; T04-F01B; U21-A05D
L65 ANSWER 8 OF 18 WPIX (C) 2003 THOMSON DERWENT
AN 2001-565624 [63] WPIX
DNN N2001-421100
TI Graphically analyzing at least one function considered in
multi-dimensional domain by projecting discrete data set on 2D and
3D planes to yield details of discrete data set's multidimensional
configuration for graphical analysis.
DC T01 T04
IN SEVASTYANOV, V
PA (SEVA-I) SEVASTYANOV V
CYC 43
PI WO 2001067395 A1 20010913 (200163)* EN 73p G06T011-20
RW: AT BE CH CY DE DK ES FI FR GB GR IE IT LU MC NL PT SE TR
W: AU BG BR BY CA CN CR CZ HU ID IL IN JP KR MX NO NZ PL RO RU SG ZA
ZW

AU 2001045377 A 20010917 (200204) G06T011-20
 US 2002015051 A1 20020207 (200213) G06T011-20
 US 6417852 B2 20020709 (200253) G06T011-20
 ADT WO 2001067395 A1 WO 2001-US6536 20010228; AU 2001045377 A AU 2001-45377
 20010228; US 2002015051 A1 Provisional US 2000-188336P 20000309, US
 2001-766462 20010119; US 6417852 B2 Provisional US 2000-188336P 20000309,
 US 2001-766462 20010119
 FDT AU 2001045377 A Based on WO 200167395
 PRAI US 2001-766462 20010119; US 2000-188336P 20000309
 IC ICM G06T011-20
 AB WO 200167395 A UPAB: 20011031

NOVELTY - A **set** of **points** is produced in a multi-
dimensional domain by device of a distributed sequences (DS)
 generator. Values of at least one function is calculated for each
point of the DS and for creating an approximation of the function
 by a discrete data **set**. The discrete data **set** is
 projected on a number of two- and **three-dimensional**
 planes to yield details of the discrete data **set**'s
 multidimensional configuration for graphical analysis.

USE - For multidimensional data analysis and visualization, for
 graphical analysis of the data set.

ADVANTAGE - Can be analyzed on the entire multidimensional domain
 without the necessity to artificially reduce **dimension** of the
 domain by assigning constant values to some of the function's parameters.
 Can use two-or **three-dimensional** projections of n-
dimensional domain without losing any information. Allows one to
 find a combination of axes for every particular chart that visualizes the
 functions' behavior as a pattern. Introduces split-criteria dividing the
 approximating data **set** into two or more **subsets** and to
 color **points** of each **subset** differently, thus making a
 specific function's behavior visible graphically. Creates an unlimited
 number of different split-criteria, and each one will generate a new
 method of graphical analysis.

DESCRIPTION OF DRAWING(S) - The drawing is a flowchart of graphical
 analysis operation according to the present invention.
 Dwg.6/19

FS EPI
 FA AB; GI
 MC EPI: T01-C04B; T01-J10C2; **T01-J10C4**; T04-H

L65 ANSWER 9 OF 18 WPIX (C) 2003 THOMSON DERWENT
 AN **2001-234039** [24] WPIX
 DNN **N2001-167268**

TI Computer implemented structure display method for medical applications,
 involves extruding display data set which is **subset** of analyzed
 image data set representing **three-spatial dimensions**
 both including data.

DC S03 S05 **T01** T04
 IN MALZBENDER, T
 PA (HEWP) HEWLETT-PACKARD CO
 CYC 1

PI US 6166740 A 20001226 (200124)* 12p G06T015-30 <--
 ADT US 6166740 A US 1994-228050 19940415
 PRAI US 1994-228050 19940415
 IC ICM **G06T015-30**
 AB US 6166740 A UPAB: 20010502

NOVELTY - The image data **set** is analyzed to determine a
set of medial axis **points** of structure extending through
three-spatial dimensions. The display data which is
subset of image data **set** is extruded by defining an
 extrusion vector in **three-spatial dimensions**. Display
set is defined to include data from image data **set** that
 lies within **set** of vector that are parallel to extrusion vector

and passes through medial axis **points**.

DETAILED DESCRIPTION - The image data set and display data set includes data representing **three-spatial dimensions**.

An INDEPENDENT CLAIM is also included for display system structure.

USE - For viewing **three-dimensional** data for extracted structure, e.g. for viewing magnetic resonance imaging (MRI) data for diagnosis and treatment of blockages existing in patient's coronary arteries.

ADVANTAGE - Provides visualization technique that is suitable for visualizing structures which has been tracked in **three-dimensional** data, hence tracked structures are enabled to be easily and readily viewed on a computer display monitor.

DESCRIPTION OF DRAWING(S) - The figure shows the flowchart explaining structure displaying method.

Dwg.3/8

FS

EPI

FA

AB; GI

MC

EPI: S03-E07A; S05-D02B2; T01-C04; T01-J06A; **T01-J10C4**; T04-H

L65

ANSWER 10 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN

2001-049881 [06] WPIX

DNN

N2001-038232 DNC **C2001-013716**

TI

Determining **three dimensional** structure of polypeptide or nucleic acid molecules, by use of an integrated technique of determining physical distance constraints and analysis of constraint information.

DC

B04 S03

IN

DOLLINGER, G; GIBSON, B W; HEMPEL, J C; KUNTZ, I D; OSHIRO, C M; TANG, N; TAYLOR, E

PA

(REGC) UNIV CALIFORNIA

CYC

93

PI

WO 2000072004 A2 20001130 (200106)* EN 80p G01N033-00

RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
NL OA PT SD SE SL SZ TZ UG ZW

W: AE AG AL AM AT AU AZ BA BB BG BR BY CA CH CN CR CU CZ DE DK DM DZ
EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK
LR LS LT LU LV MA MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI
SK SL TJ TM TR TT TZ UA UG UZ VN YU ZA ZW

AU 2000052989 A 20001212 (200115) G01N033-00

EP 1277050 A2 20030122 (200308) EN G01N033-00

R: AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE

ADT WO 2000072004 A2 WO 2000-US14667 20000526; AU 2000052989 A AU 2000-52989 20000526; EP 1277050 A2 EP 2000-937870 20000526, WO 2000-US14667 20000526

FDT AU 2000052989 A Based on WO 200072004; EP 1277050 A2 Based on WO 200072004

PRAI US 1999-135891P 19990526

IC

ICM G01N033-00

AB

WO 200072004 A UPAB: 20010126

NOVELTY - Determining the tertiary structure of a macromolecule (I) involves (M1) imposing physical distance constraints between residues of (I), fragmenting (I) into smaller molecular fragments, subjecting the fragments to an identification procedure, and then analyzing the obtained identification information to provide **three-dimensional** (3D) structural information on (I).

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:

(1) a system (II) for determining structural details of a molecule, comprises a mass spectrometer and a computational system (III) that accepts input data from the mass spectrometer, the input data comprising mass information from actual fragments of the molecule, in which the molecule has had a distance constraint imposed on it, and the computational system outputs the structural details of the molecule after matching the input data with expected fragments of the molecule that have been generated or stored by the computational system;

(2) a (III) for determining structural details of a molecule comprises one or more processors and one or more user input devices. (III) accepts input data comprising mass information from actual fragments of the molecule which has had a distant constraint imposed on it, and outputs structural details of the molecule after comparing the input data with the expected fragments of the molecule;

(3) a method implemented on (III) for scoring candidate structures of a molecule (M2) involves accepting input data, generating or storing expected fragments of the molecule, matching the mass information to the expected fragments of the molecule to generate distance constraint information and scoring the candidate structures based on how well they fit the distance constraint information; and

(4) a computer program product (IV) comprising a computer readable medium and program instructions which comprises instructions for scoring candidate structures of a molecule, provided via the computer readable medium. The program instructions specifying: accepting input data, the input data comprising mass information from actual fragments of the molecule, in which the molecule has had a distance constraint imposed on it, generating or storing expected fragments of the molecule, matching the mass information to the expected fragments of the molecule to generate distance constraint information, and scoring the candidate structures based on how well they fit the distance constraint information.

USE - For determining 3D structure or conformation of a protein or other macromolecule (a nucleic acid) (claimed), and to determine structural aspects of other macromolecules e.g. structural relationships of RNA, DNA and/or relationship of interactions of these molecules with proteins and for analyzing the results of genomic and proteomic studies.

ADVANTAGE - The method is fast, efficient as compared to conventional 3D analytical methods, and is applicable to intrinsically heterogeneous proteins such as glycosylated proteins. The protein to be studied does not need to be as pure as NMR or X-ray crystallography. Also, less protein (preferably dilute) is needed for analysis. The method is applicable to essentially all proteins.

DESCRIPTION OF DRAWING(S) - The figure shows a flow chart illustrating the integral steps of the novel method for determining tertiary structure of a macromolecule.

Dwg.1/22

FS CPI EPI

FA AB; GI; DCN

MC CPI: B04-C01; B04-E01; B11-C09

EPI: S03-E14H9

TECH

UPTX: 20010126

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Method: (M1) is carried out for determining the tertiary structure of a protein which involves reacting a protein to be analyzed with at a crosslinking reagent comprised of two reactive groups separated by a distance of from about 5-20Angstrom, and a detectable label to obtain a reaction product, enriching the reaction product for molecules having intramolecular crosslinks by subjecting the reaction product to size separation using chromatography, carrying out proteolysis on the enriched reaction product to yield protein fragments and isolating away a portion of reaction product which remains bound to a detectable label of the crosslinking reagent, subjecting the protein fragments comprising detectable labels to peptide identification analysis by mass spectroscopy and analyzing information obtained from the peptide identification analysis to provide information on the 3D structure of the (I) which is carried out by computing the mass of possible reaction products and comparing such to actual experimental masses to provide information relating to 3D structure of the amino acid sequence. The crosslinking reagent is a bifunctional crosslinker and is an amine-specific homobifunctional crosslinker. Preferably, the protein is reacted with several crosslinking agents having different specificities for reactive sites on the protein and varying

length between the reactive groups. The reaction with the crosslinker is optimized to produce an average number of one crosslinker modification per macromolecule. The reaction product obtained after reacting the protein with the crosslinking reagent is enriched for molecules having intramolecular crosslinks by physical removal proteins having intermolecular crosslinks. The peptide identification analysis is preferably by reverse-phase chromatographic separation using C4, C8 and C18 separation schemes, and mass spectrometric analysis which is carried out using matrix-assisted laser desorption ionization (MALDI) time-of-flight (TOF) instrumentation or electrospray ionization (ESI) TOF instrument. Alternately, the peptide identification analysis is comprised of peptide sequencing, by Edman sequencing method. The step of analyzing information comprises assigning values to the proteolyzed products based on mass spectrometric data, generating hypothetical structures by comparing (I) to related compounds of known structure and evaluating the hypothetical structures by considering distance constraints obtained from crosslinking data. The method further involves conducting homology modeling analysis of hypothetical structures which fit the distance constraints and choosing hypothetical structures which best fit the distance constraints. Assigning values is carried out by constructing a virtual library of proteolyzed products and which library is indexed by a criteria of monoisotopic data or average mass data. The hypothetical structures are preferably generated using a threading program for fold prediction and through use of an equation (E1) as given in the specification, where E_t is the total constraint error, d_{ij} is the pairwise distance separation, d_i is the pairwise distance defined by the structure by constraint j and i is the total number of distance constraints. The homology modeling analysis is carried using a threading alignment to match components of (I) to spatial positions of those components in a structure of (I).

TECHNOLOGY FOCUS - COMPUTING AND CONTROL - Preferred System: (II) is useful for determining structural details of a polypeptide or nucleic acid. The distance constraint (less than about 20) is imposed on the molecule by a polypeptide crosslinker such as BS3. The molecule is preferably a polypeptide and the number of distance constraints is less than 20% of the number of amino acid residues in the polypeptide. (III) in (II) accepts input data from MALDI or ESI mass spectrometer. The candidate structures of the molecules output by (III) are generated by constraint threading of a primary sequence through known protein fold. The structural details of the molecule comprise tertiary structure information and comprise a 3D coordinate map which is determined to within 2-5Angstrom RMS (**root mean square**) of the actual location of each of the atoms of the molecule. The structural details are preferably generated by homology modeling.

Preferred Method: In (M2), the candidate structures are determined to a secondary structure leveled. The method further involves generating and outputting structural details of the molecule which comprise tertiary structure information and a 3D co-ordinate map.

Preferred Computer Program: The program instructions of (IV) specify scoring candidate structures generated by constraint threading of a primary sequence through a known protein fold and further involves generating and outputting structural details of the molecule which comprise a 3D coordinate map.

ABEX

UPTX: 20010126

EXAMPLE - No relevant example is given.

L65 ANSWER 11 OF 18 WPIX (C) 2003 THOMSON DERWENT
 AN 1999-570766 [48] WPIX
 CR 2002-424771 [45]
 DNN N1999-420477 DNC C1999-166577
 TI Predicting the folded structure of proteins.
 DC B04 D16 J04 S03 T01
 IN BENNER, S A

PA (BENN-I) BENNER S A

CYC 1

PI US 5958784 A 19990928 (199948)* 113p G01N033-00

ADT US 5958784 A US 1992-857224 19920325

PRAI US 1992-857224 19920325

IC ICM G01N033-00

ICS G06F015-00

AB US 5958784 A UPAB: 20020717

NOVELTY - Predicting the folded structure of proteins, by aligning sequences of homologous proteins and using patterns of evolutionarily conserved and varied sequences to assign positions, is new.

DETAILED DESCRIPTION - This method is used for predicting the folded structure of proteins, comprising aligning the sequences of homologous proteins, using patterns of conservation and sequence variation with clearly defined evolutionary relationships. Positions in the alignment are assigned to the surface or inside of the folded structure, active sites, and parsing segments. Secondary structural units are assigned by identifying periodicity in the assignments, and assembled into globular form using distance constraints imposed by disulfide bridges, active site assignments and co-variation analysis.

An INDEPENDENT CLAIM is also included for a method predicting the secondary structure of proteins using the above method up to the point of assigning secondary structural units.

USE - The predicted secondary structures are useful for identifying antigenic sites on a protein molecule, as guides for site directed mutagenesis studies, and for understanding the interaction of a protein with other molecules.

ADVANTAGE - The method is more efficient than prior art methods of predicting folded structure of proteins.

Dwg.0/28

FS CPI EPI

FA AB; DCN

MC CPI: B04-N04; B11-C08E; B12-K04E; D05-H09; J04-B01

EPI: S03-E14; T01-J

TECH UPTX: 19991122

TECHNOLOGY FOCUS - BIOTECHNOLOGY - Essential features: Essential features of the method are:

(i) examining aligned sequences of several homologous proteins rather than a single sequence of a single protein;

(ii) extracting information concerning the **three dimensional** structure of the protein family from patterns of conservation and variation within a set of homologous sequences, rather than by a simple averaging of a property of the sequences taken individually;

(iii) combining algorithms that assign positions in the alignment to the surface or interior of the folded structure, and to the active site, as a first step for predicting secondary structural elements;

(iv) identifying separate secondary structural elements in the alignment, using parsing algorithms that identify gaps in the alignment and specific parsing sequence motifs;

(v) the algorithms are applied to **subgroups** of proteins with clearly identified evolutionary relationships, in particular a clearly specified sequence identity and evolutionary distance;

(vi) the algorithms are designed to reflect how natural selection and neutral drift influence the divergent evolution of protein sequences; and
(vii) assembling the secondary structural elements to form super secondary and tertiary structural models by orienting these elements using disulfide bridges, active site assignments and co-variation analysis.

ABEX UPTX: 19991122

EXAMPLE - The method was used to predict the structure of protein kinases, a large family of almost 100 homologous proteins. An alignment was made of the sequences of the catalytic domains of a set of protein kinases. The alignment was divided into **subgroups**. Parses, surface positions,

interior positions and active site positions were then assigned. The sequence was then divided into segments using parsing algorithms. Given the large number of sequences in the alignment, the first parsing phase could be executed using only the strongest parsing algorithm. Weaker parses were used when the individual segments were analyzed while assigning secondary structure. Details of the 14 primary parses used are given in the specification. Surface positions were then identified by the presence of variation in more than one **subgroup** at different levels of minimum pairwise identities. Interior positions were then assigned using algorithms as detailed in the specification. Active site positions were assigned to every position in the alignment where a functionalized side chain (C,D,E,H,K,N,Q,R,S,T) is conserved across the entire alignment. The data was then used to construct secondary structure hypotheses for parsed segments of the alignment. Detailed discussions and Helix wheels for each of the 15 segments of the alignment created by the primary parses are given in the specification. Assembly of the secondary structural elements to form super secondary structure requires that distances in the polypeptide chain be brought together in a **three-dimensional** space. This can be achieved by bringing together positions assigned to the active site. The large size of the protein kinase active site means that distance constraints are not very demanding. However active sites at positions 46, 113, 116, 156-62, 182, 199, 201, 210 and 305 have been used to assemble the proposed structure shown. Protein kinases lack sulfide bonds that might provide distance constraints connecting non-active sites of the protein, and no knowledge of the biochemistry of protein kinases has been used to construct the model, which is therefore incomplete.

L65 ANSWER 12 OF 18 WPIX (C) 2003 THOMSON DERWENT
 AN 1998-416200 [36] WPIX
 DNN N1998-324045
 TI Geometric object display method for computer aided design system - involves outputting geometric elements in each **sub-group** in accordance with scheduled display sequence of each **sub-group**.
 DC T01
 IN ISHIDA, T; NONAKA, S; TANAKA, Y; UNUMA, M; USAMI, Y; YOSHINAGA, T
 PA (HITA) HITACHI LTD
 CYC 28
 PI EP 858054 A2 19980812 (199836)* EN 22p G06T011-20
 R: AL AT BE CH DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO
 SE SI
 JP 10222691 A 19980821 (199844) 12p G06T015-00 <--
 CN 1193153 A 19980916 (199905) G06T015-20 <--
 KR 98071132 A 19981026 (199953) G06F017-00
 US 6075539 A 20000613 (200035) G06F015-00
 JP 3395558 B2 20030414 (200328) 12p G06T015-00 <--
 ADT EP 858054 A2 EP 1998-101738 19980202; JP 10222691 A JP 1997-25031
 19970207; CN 1193153 A CN 1998-105949 19980207; KR 98071132 A KR 1998-3415
 19980206; US 6075539 A US 1998-19195 19980205; JP 3395558 B2 JP 1997-25031
 19970207
 FDT JP 3395558 B2 Previous Publ. JP 10222691
 PRAI JP 1997-25031 19970207
 REP No-SR.Pub
 IC ICM G06F015-00; G06F017-00; G06T011-20; G06T015-00;
 G06T015-20
 ICA G06F017-50
 AB EP 858054 A UPAB: 19980911
 The method involves deriving geometric element data from a data source of geometric elements to be finally displayed (1201). In accordance with the derived geometric element data, displaying a geometric element contained in each of all the groups to be displayed finally, until 50 % of all the geometric elements to be finally displayed is displayed. Geometric element

data of the geometric object to be displayed are inputted. The geometric elements contained in each group of the input geometric element data are **sub-grouped** into a plurality of **sub-groups**. The display sequence of the **sub-groups** of each group is scheduled. The geometric elements in each **sub-group** is outputted in accordance with the scheduled display sequence of each **sub-group**.

ADVANTAGE - Makes it easy to grasp outline of composite geometric object at earlier stage while only partial geometric element data is displayed.

Dwg.2/18

FS

EPI

FA

AB; GI

MC

EPI: T01-J10C; T01-J15A

L65 ANSWER 13 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 1997-193099 [17] WPIX

DNN N1997-159461

TI Method isolating anatomical structures in **3 dimensional** dataset - uses fuzzy connectivity to define data points of desired structure to reconstruct only desired structure, helps its viewing & analysis, uses recursive opening & erosion of **3D** dataset to form skeleton to form residuals for skeleton.

DC S05 T01

IN KRASKE, W F

PA (NOTH) NORTHROP GRUMMAN CORP

CYC 71

PI WO 9709690 A1 19970313 (199717)* EN 85p G06K009-00.

RW: AT BE CH DE DK EA ES FI FR GB GR IE IT KE LS LU MC MW NL OA PT SD
SE SZ UG

W: AL AM AT AU AZ BB BG BR BY CA CH CN CZ DE DK EE ES FI GB GE HU IL
IS JP KE KG KP KR KZ LK LR LS LT LU LV MD MG MK MN MW MX NO NZ PL
PT RO RU SD SE SG SI SK TJ TM TR TT UA UG UZ VN

AU 9669174 A 19970327 (199729) G06K009-00

TW 357325 A 19990501 (199937) G06T017-00 <--

ADT WO 9709690 A1 WO 1996-US14500 19960905; AU 9669174 A AU 1996-69174
19960905; TW 357325 A TW 1996-115555 19961217

FDT AU 9669174 A Based on WO 9709690

PRAI US 1995-523438 19950905

REP 1.Jnl.Ref; US 5201011

IC ICM G06K009-00; G06T017-00

ICS G06K009-40

AB WO 9709690 A UPAB: 19970424

The method forms a morphological skeleton of the **3 dimensional** dataset and selects a seed data point within the morphological skeleton. The point being contained in the desired anatomical structure.

Fuzzy connectivity is used to define additional data **points** of the desired structure to reconstruct only the desired structure. The reconstruction facilitates the viewing and analysis of it. Recursive opening and erosion of the **3 dimensional** data **set** is used to form the skeleton to form several residuals defining the skeleton.

USE/ADVANTAGE - Relates to medical imaging systems and digital signal processing and to use of data dimensional sieving and fuzzy connectivity to facilitate analysis and review of **3 dimensional** medical images such as those produced by magnetic resonance imaging devices and similar. Specifically addresses and alleviates deficiencies with existing equipment.

Dwg.0/14

FS

EPI

FA

AB

MC

EPI: S05-D02B2; S05-D02C; T01-J16B; T01-S01B

L65 ANSWER 14 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 1996-277253 [28] WPIX

DNN N1996-233285

TI Computer number of varying data displaying - displaying is produced in first or inner coordinate system corresp to first **subset** of given variables and placing of resulting display in second or outer coordinate system.

DC T01

IN BESHES, C M; FEINER, S K

PA (UYCO) UNIV COLUMBIA NEW YORK

CYC 1

PI US 5524187 A 19960604 (199628)* 13p G06F015-62

ADT US 5524187 A Cont of US 1991-675579 19910325, US 1994-299812 19940901

PRAI US 1991-675579 19910325; US 1994-299812 19940901

IC ICM G06F015-62

AB US 5524187 A UPAB: 19960719

The method involves first computing based on computer input of the multiple variable data, for forming a first, **3-dimensional** display in a first coordinate system corresp to a first **subset** of variables. A second computing is based on the computer input of the multiple variable data and dependent on the first computer processing.

Such arrangement is for displaying the first display in a second coordinate system corresp to a second **subset** of variables such that a designated **point** of the first coordinate system is located at a **point** in the second coordinate system. E.g. the coordinates of the **point** in the second coordinate system fix a **set** of variables that are used in determining the first display. A third computing is used for manipulating the first display by geometric transformation.

USE/ADVANTAGE - For developing true **3-D** interaction device. Facilitated display and manipulation of nested coordinate system by use of **3D** window system capable of organising and displaying **3D** spatial regions in oriented tree structure.

Dwg.2/6

FS EPI

FA AB; GI

MC EPI: T01-J10C1; T01-J10C4

L65 ANSWER 15 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 1995-014436 [02] WPIX

DNN N1995-011271

TI Display pixels vector-based terms normalisation - determining **square** of magnitude of vector associated with each vector-based term for each pixel from preset vectors at vertices of polygon, with approximation of reciprocal of **square root** using series expansion.

DC T01

IN ASSARPOUR, H; GHOLIZADEH, D; MESSAOUDENE, M

PA (DIGI) DIGITAL EQUIP CORP

CYC 1

PI US 5369737 A 19941129 (199502)* 14p G06F015-62

ADT US 5369737 A Cont of US 1988-170749 19880321, Cont of US 1989-405104 19890908, US 1990-568529 19900815

PRAI US 1988-170749 19880321; US 1989-405104 19890908; US 1990-568529 19900815

IC ICM G06F015-62

ICS G06F015-72

AB US 5369737 A UPAB: 19950117

Vector-based terms are normalised for display pixels associated with a polygon representing a surface of an object being imaged. The

vector-based terms are determined from predetermined vectors at vertices of the polygon. The square (η) of the magnitude of a vector associated with each vector-based term is determined for each display pixel from the predetermined vectors at the vertices of the polygon.

The quantity $1/(\text{square root } \eta)$ is approximated for each vector-based term using a series expansion employing η , and each vector based term is multiplied by the corresponding approximation of $(1/\text{square root } \eta)$ to produce a normalised vector-based term for each display pixel.

Dwg.1/4

FS

EPI

FA

AB; GI

MC

EPI: T01-J10B2; T01-J10C4

L65

ANSWER 16 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN

1994-360300 [45] WPIX

DNN

N1994-282343

TI

Image synthesis system for generating parametric curve - generates interpolated values using phantom control values, determined by combining respective **subsets** of received control values in accordance with set of coefficients used repeatedly and combined with **subset** of received control values.

DC

T01 T06 X25

IN

MCINALLY, T C

PA

(CANO) CANON KK; (CANO) CANON RES CENT EURO LTD

CYC

4

PI

GB 2278470	A	19941130 (199445)*	94p	G06F015-353
EP 626648	A1	19941130 (199501)	EN 34p	G06F015-353
R: DE FR GB				

US 5608856	A	19970304 (199715)	31p	G06T011-00
GB 2278470	B	19971224 (199803)		G06F017-17
EP 626648	B1	20001004 (200050)	EN	G06F017-17
R: DE FR GB				

DE 69426042	E	20001109 (200064)		G06F017-17
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ADT

GB 2278470 A GB 1993-11157 19930528; EP 626648 A1 EP 1994-303771 19940525; US 5608856 A US 1994-249910 19940526; GB 2278470 B GB 1993-11157 19930528; EP 626648 B1 EP 1994-303771 19940525; DE 69426042 E DE 1994-626042 19940525, EP 1994-303771 19940525

FDT

DE 69426042 E Based on EP 626648

PRAI

GB 1993-11157 19930528

REP

05Jnl.Ref

IC

ICM G06F015-353; G06F017-17; G06T011-00

ICS G06T015-10

AB

GB 2278470 A UPAB: 19950102

A definer/editor stores object definitions in the form of control **points** for spline curves. The system can generate phantom control **points** (AO to AN+1) to define a spline object, such that the curve interpolates a desired **set of points** (P1 to PN) received from a user, for example via a mouse or graphics tablet.

USE/ADVANTAGE - E.g. for computer aided design, robotics, numerical control, and picture and motion picture recordings. While number N of received **points** is variable, and may be large, system operates quickly to generate coefficients (X_{ij}) which can be used to derive phantom control **points** (A), without need for matrix inversion, and without storing large number of pre-inverted matrices, to permit intuitive interaction with user for definition of spline objects. For large numbers N where interactivity may become difficult to achieve, system generates approximate phantom **points**, each derived from small **sub-set** of received **points**.

Dwg.3a/17

FS

EPI

FA

AB; GI

MC

EPI: T01-J10C2; T01-J15; T06-A04A; T06-A07A; T06-D07B; X25-A03E; X25-A03F

ABEQ US 5608856 A UPAB: 19970410

A computer graphics apparatus for generating image data representing a graphic object having a curved shape, the curved shape approximately interpolating a **set** of N control **points**, comprising:

means for receiving electrical signals defining the **set** of N control **points**;

processing means for processing the electrical signals to generate a **set** of phantom control **points**, comprising means for combining respective **subsets** of N (fewer than N) of the control **points** in accordance with a **set** of N coefficients, such that the **set** of N coefficients is used repeatedly and combined with a respective different **subset** of the control **points** to generate each of at least a middle **subset** of the phantom control **points**;

means for storing the **set** of phantom control **points** generated by the processing means as part of an object database for subsequent use in generating the image data;

generating means for generating one or more interpolated points by using the phantom control points stored in the object database in a parametric equation, so as to generate the image data, the interpolated points representing the curved shape of the object.

Dwg.11/17

ABEQ GB 2278470 B UPAB: 19980119

A definer/editor stores object definitions in the form of control **points** for spline curves. The system can generate phantom control **points** (AO to AN+1) to define a spline object, such that the curve interpolates a desired **set** of **points** (P1 to PN) received from a user, for example via a mouse or graphics tablet.

USE/ADVANTAGE - E.g. for computer aided design, robotics, numerical control, and picture and motion picture recordings. While number N of received **points** is variable, and may be large, system operates quickly to generate coefficients (Xij) which can be used to derive phantom control **points** (A), without need for matrix inversion, and without storing large number of pre-inverted matrices, to permit intuitive interaction with user for definition of spline objects. For large numbers N where interactivity may become difficult to achieve, system generates approximate phantom **points**, each derived from small **sub-set** of received **points**.

L65 ANSWER 17 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 1991-045874 [07] WPIX

CR 1989-159240 [22]; 1992-133873 [17]; 1994-117852 [14]

DNN N1991-035733

TI 3-Dimensional generating method image from 2-dimensional slice images - allowing 3-dimensional image to be generated quickly by minimising number of calculation required.

DC S05 T01

IN KROCHTA, T J; TUY, H K; LIN, H; MAILEY, F C

PA (PXR) PICKER INT INC

CYC 5

PI EP 412748 A 19910213 (199107)*

R: DE FR GB NL

US 5079699 A 19920107 (199205)

US 5170347 A 19921208 (199252)# 34p G06F015-42

EP 412748 A3 19930127 (199347)

EP 412748 B1 19970226 (199714) EN 16p G06T015-00 <--

R: DE FR GB NL

DE 69029982 E 19970403 (199719)

G06T015-00 <--

ADT EP 412748 A EP 1990-308618 19900806; US 5079699 A US 1989-391484 19890809; US 5170347 A CIP of US 1987-126368 19871127, Cont of US 1988-200697 19880531, US 1990-517388 19900430; EP 412748 A3 EP 1990-308618 19900806; EP 412748 B1 EP 1990-308618 19900806; DE 69029982 E DE 1990-629982

19900806, EP 1990-308618 19900806
 FDT US 5170347 A CIP of US 4882679; DE 69029982 E Based on EP 412748
 PRAI US 1989-391484 19890809; US 1987-126368 19871127; US 1988-200697
 19880531; US 1990-517388 19900430
 REP NoSR.Pub; 1.Jnl.Ref; EP 265334; EP 318176; US 4879652; JP 01119786
 IC ICM G06F015-42; **G06T015-00**
 ICS G06F015-72
 AB EP 412748 A UPAB: 19960405

The method involves defining a region of interest from a boundary and extrapolating it in to slices. Pixels representative of the boundary of interest are isolated and represented by three vectors having equivalent entries in each. First and second vectors store data representative of the coordinates for pixels within each slice. Entries in the third vector correspond to physical properties of a specimen at a location defined by corresp. entries in the first and second sectors.

A linear extrapolation between respective elements of a lengthened vector and the larger of the vectors is made. Then linear interpolation of the intermediated vector to a number of vector elements intermediate the larger and smaller of the neighbouring vectors is made. This process is continued during a preselected number of iterations. The method is completed with the mapping of all sets of first, second and third vectors to pixels of an associated picture frame.

USE/ADVANTAGE - For medical diagnostic purposes. Fast response time.
 @ (14pp Dwg.No.7/9)@
 7/9

FS EPI
 FA AB; GI
 MC EPI: S05-D02A1; S05-D02X; T01-J06A; T01-J10C
 ABEQ US 5079699 A UPAB: 19930928

The diagnostic imaging system generates a **three-dimensional** display from a series of two-dimensional slice images. A region of interest, defined from a boundary of interest, is selected from one slice and is extrapolated to subsequent slices. Pixels representative of the boundary of interest are isolated and represented by **three** vectors having an equivalent entries in each. First and second vectors store data representative of first and second coordinates for pixels within each slice. Entries in the **third** vector correspond to physical properties of a specimen at a location defined by corresponding entries in the first and second vectors. Areas representative of boundaries of interest falling between slices are extrapolated from vector data from slices neighbouring the area.

This is accomplished by a linear interpolation of elements of the set of smaller vectors to a number equivalent to the entries in the neighbouring larger vectors. Next, a linear extrapolation between respective elements of the lengthened vector and the longer of the vector is made. Finally, a linear interpolation of the intermediate vector to a number of vector elements intermediate the larger and smaller of the neighbouring vectors is made. This process is suitably continued during a preselected number of iterations. Finally, a discretised **three-dimensional** object represented by all sets of first, second and **third** vectors are mapped to pixels of an associated pixel frame.

USE - E.g. for CT scanner.

ABEQ US 5170347 A UPAB: 19930928

The system for **three-dimensional** diagnostic imaging generates slice images of a specimen. A region of interest is selected from within a slice and is extrapolated to subsequent slices. A boundary indicative of a surface of interest is selected from within the region of interest to facilitate generation of an image representative of a **three-dimensional** surface of interest to be assembled from subsequent slices. A viewing surface is defined in relation to a generated surface image which was selected from the boundary.

A scaler assigns a scaled grey level to the **three**-dimensional image to facilitate **three-dimensional**

viewing of the object when it is projected on the viewing surface. Image information is selectably modified by data from the original slice images to add surface density visualisation.

USE/ADVANTAGE - CT scanners, adaptable to general purpose processors, increased fidelity and resolution, enhanced visualisation of surface density of **3-D** images. (Dwg.5/14c
5/14c

ABEQ EP 412748 A UPAB: 19940111

The method involves defining a region of interest from a boundary and extrapolating it in to slices. Pixels representative of the boundary of interest are isolated and represented by three vectors having equivalent entries in each. First and second vectors store data representative of the coordinates for pixels within each slice. Entries in the third vector correspond to physical properties of a specimen at a location defined by corresp. entries in the first and second sectors.

A linear extrapolation between respective elements of a lengthened vector and the larger of the vectors is made. Then linear interpolation of the intermediated vector to a number of vector elements intermediate the larger and smaller of the neighbouring vectors is made. This process is continued during a preselected number of iterations. The method is completed with the mapping of all sets of first, second and third vectors to pixels of an associated picture frame.

USE/ADVANTAGE - For medical diagnostic purposes. Fast response time. @ (14pp Dwg.No.7/9)@

ABEQ EP 412748 B UPAB: 19970407

A method of generating **three-dimensional** images from a plurality of two-dimensional images comprising the steps of: acquiring a series of generally parallel image slices from an associated specimen, each slice being represented by a generally planar array of voxels, each voxel being defined by unique first and second spatial **dimensions** along the slice, and a viewing value representative of a physical characteristic of the associated specimen (40) thereat; isolating a **subset** of voxels along a boundary of interest in each slice, which boundary of interest defines a region of interest; a slice interpolation step of interpolating, from boundaries of interest of neighbouring slices, a **subset** of voxels representative of an intermediate boundary of interest displaced intermediate each of the neighbouring slices; discretizing a **three-dimensional** object of each boundary of interest of each slice such that each voxel thereof maps to a pixel of an associated picture frame; and projecting the discretized object to the picture frame, characterised by further comprising the steps of for each slice, defining a first vector array of data representative of the first coordinate of each **subset** of voxels thereof; defining a second vector array of data representative of the first coordinate of each **subset** of voxels thereof; defining a second vector array of data representative of the second coordinate of each **subset** of voxels thereof; defining a **third** vector for each **subset** of data representative of the viewing value for each **subset** of voxels thereof; and a vector interpolation step of interpolating, prior to the slice interpolation step, the boundaries of interest of neighbouring slices to equivalent lengths between corresponding first, second, and **third** vectors and interpolating between corresponding vectors of adjacent slices.
Dwg.1/9

L65 ANSWER 18 OF 18 WPIX (C) 2003 THOMSON DERWENT

AN 1979-G3757B [30] WPIX

TI **Three-dimensional** imaging system - uses groups of light sources providing sets of partial images in respective recording planes of e.g. film.

DC P31 P82 V05

IN LINDE, R; TIEMENS, U; WEISS, H

PA (PHIG) PHILIPS PATENTVERWALTUNG GMBH

CYC 4
 PI DE 2801940 A 19790719 (197930)*
 GB 2012530 A 19790725 (197930)
 FR 2417126 A 19791012 (197947)
 US 4246483 A 19810120 (198106)
 GB 2012530 B 19820519 (198220)
 PRAI DE 1978-2801329 19780113; DE 1978-2801940 19780118
 IC A61B006-02; G03B041-16; H05G001-02
 AB DE 2801940 A UPAB: 19930901

The imaging system has the **3-dimensional** object illuminated by a number of light sources (2', 2", 5', 5") positioned next to one another. Two or more **sub-groups** are selected from these light sources (2', 2", 5', 5") each used to record individual perspective images in a corresponding recording plane (4', 4") of a multi-layer recording medium (4), e.g. a film.

The recorded images are decoded one after the other or simultaneously by Tomosynthesis, in which two or more partial images of an object are superimposed. The **sub-groups** of light sources (2', 2", 5', 5") may be positioned symmetrically and they may be selected via a screen and shutter system (1", 1").

FS EPI GMPI
 FA AB

=> fil dpci
 FILE 'DPCI' ENTERED AT 10:06:50 ON 06 MAY 2003
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FILE LAST UPDATED: 30 APR 2003 <20030430/UP>
 PATENTS CITATION INDEX, COVERS 1973 TO DATE

>>> LEARNING FILE LDPCI AVAILABLE <<<

=> d all tot 166

L66 ANSWER 1 OF 4 DPCI COPYRIGHT 2003 THOMSON DERWENT
 AN 2002-487852 [52] DPCI
 CR 1993-308303 [39]; 2002-507172 [54]; 2002-607266 [65]; 2002-712495 [77]
 DNN N2002-385480 DNC C2002-138550
 TI Analyzing sequences of atomic groups by preparing memory elements corresponding to first sequence, initializing all elements to zero and obtaining longest common subsequence between chains of atomic groups.
 DC B04 D16 S03 T01
 IN AIKAWA, S; MATSUZAWA, F; TOMIKAWA, M
 PA (FUIT) FUJITSU LTD
 CYC 1
 PI US 6370479 B1 20020409 (200252)* 61p G06F019-00 <--
 ADT US 6370479 B1 US 1993-14867 19930208
 PRAI JP 1992-331703 19921211; JP 1992-21012 19920206
 IC ICM G06F019-00
 ICS G01N033-48; G01N033-50
 FS CPI EPI

EXF EXAMINER'S FIELD OF SEARCH UPE: 20030227

NCL US 6370479 B1 20020409
 000/364.496; 000/364.497; 000/364.578; 000/395.600; 000/436.630;
 000/702.190; 000/702.200; 000/702.270; 000/703.110

CTCS CITATION COUNTERS

PNC.DI 0 Cited Patents Count (by inventor)

PNC.DX	10	Cited Patents Count (by examiner)
IAC.DI	0	Cited Issuing Authority Count (by inventor)
IAC.DX	1	Cited Issuing Authority Count (by examiner)
PNC.GI	0	Citing Patents Count (by inventor)
PNC.GX	0	Citing Patents Count (by examiner)
IAC.GI	0	Citing Issuing Authority Count (by inventor)
IAC.GX	0	Citing Issuing Authority Count (by examiner)
CRC.I	0	Cited Literature References Count (by inventor)
CRC.X	6	Cited Literature References Count (by examiner)

CDP CITED PATENTS

UPD: 20030227

Cited by Examiner

CITING PATENT	CAT	CITED PATENT	ACCNO
US 6370479	B1	US 4823306	A 1989-055618/08
	PA:	(IBMC) IBM CORP; (IBMC) INT BUSINESS MACHINES CORP	
	IN:	BARBIC, F; CHOY, D M H; CHOY, D M	
		US 4853871	A 1988-307666/43
	PA:	(GEMX) GENEX CORP	
	IN:	LADNER, R C; PANTOLIANO, M W	
		US 4939666	A 1989-280747/39
	PA:	(GEMX) GENEX CORP	
		US 5157736	A 1992-373358/45
	PA:	(IBMC) INT BUSINESS MACHINES CORP	
	IN:	BOYER, S K; CASEY, R G; MILLER, A M; OUDOT, B; ZILLES, K S	
		US 5200910	A 1992-300238/36
	PA:	(STRD) UNIV LELAND STANFORD JUNIOR	
	IN:	SUBBIAH, S	
		US 5241470	A 1993-287917/36
	PA:	(STRD) UNIV LELAND STANFORD JUNIOR	
	IN:	LEE, C; SUBBIAH, S	
		US 5263159	A 1991-095848/14
	PA:	(IBMC) IBM CORP; (IBMC) INT BUSINESS MACHINES CORP	
	IN:	MITSUI, K	
		US 5331573	A 1994-234155/28
	PA:	(BALA-I) BALAJI V N; (SING-I) SINGH C U	
	IN:	BALAJI, V N; SINGH, C U	
		US 5410493	A 1992-179147/22
	PA:	(NIDE) NEC CORP	
	IN:	KONAGAYA, A	
		US 5446798	A 1991-022356/03
	PA:	(FUIT) FUJITSU LTD	
	IN:	KAWAKAMI, S; MORITA, T	

REN LITERATURE CITATIONS UPR: 20030227

Citations by Examiner

CITING PATENT	CAT	CITED LITERATURE
US 6370479	B1	Vriend and Sander, "Detection of Common Three-Dimensional Substructures in Proteins" Proteins: Structure, Function, and Genetics, No. 1, 1991, pp. 52-58.

US 6370479 B1 Alexandrov, Takahashi, and Go, "Common Spatial Arrangements of Backbone Fragments in Homologous and Non-homologous Proteins" Journal of Molecular Biology, (1992) 225, pp. 5-9.

US 6370479 B1 Shoichi Sato and Toru Yao, "Homology Analysis of Protein Conformational Data," The Tenth Chemistry Information Discussion Meeting, Nov. 6-Nov. 8, 1987, The Fifteenth Structure-Activity Relationship Program, Nov. 6-Nov. 8, 1987, pp. 88-92 (English Translation numbered as pp. 1-6).

US 6370479 B1 Toru Kitanaka and Hideaki Umeyama, "Development of a Protein Modeling Method by Using Known Conformations", The Tenth Chemistry Information Discussion Meeting, Nov. 6-Nov 8, 1987, The Fifteenth Structure-Activity Relationship Program, Nov. 6-Nov. 8, 1987, pp. 354-357 (English Translation numbered as pp. 7-15).

US 6370479 B1 Nobuo Tomioka and Akiko Itai, "A Variety of Computer Images Molecular Designing and Molecular Modeling", pp. 64, 65, et seq. (English Translation numbered as pp. 16-23).

US 6370479 B1 Orengo, Brown, and Taylor, "Fast Structure Alignment for Protein Databank Searching" Proteins: Structure, Function, and Genetics 14:139-167 (1992).

L66 ANSWER 2 OF 4 DPCI COPYRIGHT 2003 THOMSON DERWENT

AN 1997-003764 [01] DPCI

DNN N1997-003343

TI 3D structure display method for analysing substance such as protein using X-ray crystal analysis appts - involves performing character display by display type corresponding to setting of display attribute of character display unit buffer.

DC T01

IN AIKAWA, S; MATSUZAWA, F; NISHINA, S

PA (FUIT) FUJITSU LTD

CYC 2

PI JP 08272848 A 19961018 (199701)* 12p G06F017-50 <--

US 6125332 A 20000926 (200051) G06F017-00 <--

ADT JP 08272848 A JP 1995-76765 19950331; US 6125332 A US

1996-620289 19960322

PRAI JP 1995-76765 19950331

IC ICM G06F017-00; G06F017-50

ICS G06T017-00

FS EPI

EXF EXAMINER'S FIELD OF SEARCH UPE: 20001113

NCL US 6125332 A 20000926
 345/115; 345/116; 345/302; 345/340; 345/507; 364/496; 364/497; 364/498;
 364/499; 364/550; 364/578; 395/118; 395/119; 395/131; 395/133; 395/167;
 395/500.330; 395/770; 702/027; 702/032; 707/526; 707/528; 707/529; 711/101

CTCS CITATION COUNTERS

PNC.DI	0	Cited Patents Count (by inventor)
PNC.DX	7	Cited Patents Count (by examiner)
IAC.DI	0	Cited Issuing Authority Count (by inventor)
IAC.DX	2	Cited Issuing Authority Count (by examiner)
PNC.GI	0	Citing Patents Count (by inventor)
PNC.GX	0	Citing Patents Count (by examiner)

IAC.GI 0 Citing Issuing Authority Count (by inventor)
 IAC.GX 0 Citing Issuing Authority Count (by examiner)
 CRC.I 0 Cited Literature References Count (by inventor)
 CRC.X 3 Cited Literature References Count (by examiner)

CDP CITED PATENTS

UPD: 20001113

Cited by Examiner

CITING PATENT	CAT	CITED PATENT	ACCNO
US 6125332	A	JP 6180737	A
		US 4747059	A 1988-161435/23
PA:		(SUNR) SUNTORY LTD	
IN:		HIRYAMA, K; TIAZO, T	
		US 5321804	A 1994-191886/23
PA:		(FUIT) FUJITSU LTD	
IN:		ARAI, M; IMAMURA, F; KUSABA, S; TANIUCHI, K	
		US 5337402	A 1994-255602/31
PA:		(DESI-N) DESIGN AUTOMATION INC; (KITA-I) KITAGAWA K;	
		(OMRO) OMRON CORP	
IN:		KITAGAWA, K; TANI, I	
		US 5704051	A 1998-076745/07
PA:		(LANE-I) LANE M W; (LANE-I) LANE R S	
IN:		LANE, M W; LANE, R S	
		US 5708764	A 1997-026220/03
PA:		(IBMC) IBM CORP; (IBMC) INT BUSINESS MACHINES CORP	
IN:		BORREL, P; CHENG, K F; MENON, J P; ROSSIGNAC, J R	
		US 5710878	A 1997-052594/05
PA:		(VIRT-N) VIRTUAL WORLD ENTERTAINMENT INC; (ALBE-I)	
		ALBERTSON J; (MCCO-I) MCCOY D S	
IN:		ALBERTSON, J; MCCOY, D S	

REN LITERATURE CITATIONS UPR: 20001113

Citations by Examiner

CITING PATENT	CAT	CITED LITERATURE
US 6125332	A	Smith, "MolView: A Program to Analyze and Display Atomic Structures" SciTech Journal Jan., 1995 p. 24-25.
US 6125332	A	HyperChem for Windows. Reference Manual. Jul. 21, 1993 p. 4, 65-67, 77-82, 98-104, 126-127, 130-131, 135, 148-149, 153-154, 162-167, 228-231.
US 6125332	A	Introduction to Protein Structure, Branden and Tooze, Garland Publishing, Inc., 1991, pp. 3-4, 6-7 and 121.

L66 ANSWER 3 OF 4 DPCI COPYRIGHT 2003 THOMSON DERWENT

AN 1996-043514 [05] DPCI

DNN N1996-036531

TI Common structure extraction unit for extracting common features of different 3D structure - has common partial extractor to extract common portion of two point assembling based on calculated accumulation distance.

DC T01

IN AIKAWA, S; MATSUZAWA, F; TOMIKAWA, M

PA (FUIT) FUJITSU LTD

CYC 2
 PI JP 07287717 A 19951031 (199605)* 56p G06F017-30 <--
 JP 3235763 B2 20011204 (200203) 56p G06F017-30 <--
 US 6453064 B1 20020917 (200264) G06K009-00 <--
 ADT JP 07287717 A JP 1995-10805 19950126; JP 3235763 B2 JP
 1995-10805 19950126; US 6453064 B1 US 1995-390862 19950217
 FDT JP 3235763 B2 Previous Publ. JP 07287717
 PRAI JP 1994-30157 19940228
 IC ICM G06F017-30; G06K009-00
 ICS G06F017-50
 FS EPI

EXF EXAMINER'S FIELD OF SEARCH UPE: 20030401

NCL US 6453064 B1 20020917
 000/345.135; 000/345.139; 000/345.629; 000/345.630; 000/345.653;
 000/345.664; 000/345.679; 000/364.496; 000/382.128; 000/382.129;
 000/382.154; 000/382.201; 000/382.209; 000/382.216; 000/382.217;
 000/382.218; 000/382.219; 000/382.224; 000/382.225; 000/382.226;
 000/382.228; 000/382.294; 000/382.305; 000/395.113; 000/395.115;
 000/395.116; 000/395.119; 000/702.190

CTCS CITATION COUNTERS

PNC.DI	0	Cited Patents Count (by inventor)
PNC.DX	10	Cited Patents Count (by examiner)
IAC.DI	0	Cited Issuing Authority Count (by inventor)
IAC.DX	2	Cited Issuing Authority Count (by examiner)
PNC.GI	0	Citing Patents Count (by inventor)
PNC.GX	0	Citing Patents Count (by examiner)
IAC.GI	0	Citing Issuing Authority Count (by inventor)
IAC.GX	0	Citing Issuing Authority Count (by examiner)
CRC.I	0	Cited Literature References Count (by inventor)
CRC.X	6	Cited Literature References Count (by examiner)

CDP CITED PATENTS UPD: 20030401

Cited by Examiner

CITING PATENT	CAT	CITED PATENT	ACCNO
JP 3235763	B2	JP 4045781 A	1992-101933/13
	PA:	(FUIT) FUJITSU LTD	
		JP 5219932 A	1993-308303/39
	PA:	(FUIT) FUJITSU LTD	
		JP 62044897 A	
		JP 63259598 A	
US 6453064	B1	JP 4045781 A	1992-101933/13
	PA:	(FUIT) FUJITSU LTD	
		JP 5219932 A	1993-308303/39
	PA:	(FUIT) FUJITSU LTD	
		JP 62044897 A	
		JP 63259598 A	
		US 4881175 A	1990-030146/04
	PA:	(GENE) GENERAL ELECTRIC CO	
	IN:	LADNER, R C	
		US 5025388 A	1991-200832/27
	PA:	(TRIP-N) TRIPOS ASSOC INC; (CRAM-I) CRAMER R D;	

(WOLD-I) WOLD S; (SVAN-I) SVANTE W
 IN: CRAMER, R D; WOLD, S B; WOLD, S V; SVANTE, W
 US 5058200 A 1991-324845/44
 PA: (GENE) GENERAL ELECTRIC CO
 IN: HUANG, C C; PUCKETTE, C M
 US 5265030 A 1991-340015/46
 PA: (SCRI) SCRIPPS CLINIC & RES FOUND; (SCRI-N) SCRIPPS
 CLINIC & RE
 IN: SKOLNICK, J; KOLINSKI, A
 US 5436850 A 1993-045645/05
 PA: (REGC) UNIV CALIFORNIA
 IN: BOWIE, J U; EISENBERG, D; LUTHY, R
 US 5568384 A 1996-485321/48
 PA: (MAYO-N) MAYO FOUNDATION
 IN: JIANG, H; ROBB, R A

REN LITERATURE CITATIONS UPR: 20030401

Citations by Examiner

CITING PATENT	CAT	CITED LITERATURE
US 6453064	B1	Itai et al., "Present state of the medicine molecular design using the computer", Pharmacy Library, vol. 36, No. 1, 1991, pp. 10-23.*
US 6453064	B1	Vriend et al.; "Detection of Common Three-Dimensional Substructures in Proteins"; Proteins, Structure, Function, and Genetics; No. 1, 1991.*
US 6453064	B1	Itai & Tomioka; "Computer Graphics Directing to Lead Generation"; Extra Issue of "Contemporary Chemistry", vol. 13, 1987, pp. 57-72.*
US 6453064	B1	Alexandrov et al.; Common Spatial Arrangements of Backbone Fragments in Homologous and Non-homologous Proteins; Journal of Mol. Biol., vol. 225, No. 1, May 5, 1992.*
US 6453064	B1	N. Alexandrov et al., "Common Spatial Arrangements of Backbone Fragments in Homologous and Non-homologous Proteins", Journal of Molecular Biology, vol. 25, No. 1, 1992, pp. 5-9.*
US 6453064	B1	G. Vriend et al., "Detection of Common Three-Dimensional Substructures in Proteins", European Molecular Biology Laboratory, 1991, pp. 52-58.

L66 ANSWER 4 OF 4 DPCI COPYRIGHT 2003 THOMSON DERWENT
 AN 1993-308303 [39] DPCI
 CR 2002-487852 [52]; 2002-507172 [54]; 2002-607266 [65]; 2002-712495 [77]
 DNN N1993-237572 DNC C1993-136720
 TI Gene information testing device to evaluate similarity between aminoacid sequence and reference aminoacid - comprises unit to detect number of longest common letter between the sequences and calculation unit to find ratio of longest common letter detected.
 DC B04 D16 J04 S03 S05 T01
 PA (FUIT) FUJITSU LTD
 CYC 1
 PI JP 05219932 A 19930831 (199339)* 17p C12M001-00 <--
 ADT JP 05219932 A JP 1992-21012 19920206
 PRAI JP 1992-21012 19920206
 IC ICM C12M001-00
 ICS G06F015-40; G06F015-42

FS CPI EPI

CTCS CITATION COUNTERS

PNC.DI	0	Cited Patents Count (by inventor)
PNC.DX	0	Cited Patents Count (by examiner)
IAC.DI	0	Cited Issuing Authority Count (by inventor)
IAC.DX	0	Cited Issuing Authority Count (by examiner)
PNC.GI	0	Citing Patents Count (by inventor)
PNC.GX	2	Citing Patents Count (by examiner)
IAC.GI	0	Citing Issuing Authority Count (by inventor)
IAC.GX	2	Citing Issuing Authority Count (by examiner)
CRC.I	0	Cited Literature References Count (by inventor)
CRC.X	0	Cited Literature References Count (by examiner)

CGP CITING PATENTS UPG: 20030401

Cited by Examiner

CITED PATENT	CAT	CITING PATENT	ACCNO
JP 5219932	A	JP 3235763	B2 1996-043514/01
	PA:	(FUIT) FUJITSU LTD	
		US 6453064	B1 1996-043514/01
	PA:	(FUIT) FUJITSU LTD	
	IN:	AIKAWA, S; MATSUZAWA, F; TOMIKAWA, M	

=> fil wpix

FILE 'WPIX' ENTERED AT 10:14:53 ON 06 MAY 2003
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FILE LAST UPDATED: 5 MAY 2003 <20030505/UP>
 MOST RECENT DERWENT UPDATE: 200329 <200329/DW>
 DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

Due to data production problems in updates 24 and 25
 the WPI file had to be reset to update 200323 on April 24
 and the corrected updates were reloaded.
 SDIs for update 24 were rerun. The previous SDI run for 24 has
 been credited.
 We also recommend to recreate answer sets dated between April 10
 and 24. Charges incurred to accomplish this will be credited of
 course.

>>> NEW WEEKLY SDI FREQUENCY AVAILABLE --> see NEWS <<<

>>> SLART (Simultaneous Left and Right Truncation) is now
available in the /ABEX field. An additional search field
/BIX is also provided which comprises both /BI and /ABEX <<<

>>> PATENT IMAGES AVAILABLE FOR PRINT AND DISPLAY <<<

>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES,
SEE <http://www.derwent.com/dwpi/updates/dwpicov/index.html> <<<>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
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>>> FOR INFORMATION ON ALL DERWENT WORLD PATENTS INDEX USER
GUIDES, PLEASE VISIT:
http://www.derwent.com/userguides/dwpi_guide.html <<<

=> d all abeq tech abex tot

L72 ANSWER 1 OF 22 WPIX (C) 2003 THOMSON DERWENT
AN 1998-076745 [07] WPIX
DNN N1998-061401
TI Hierarchical menu bar with dynamic graphics and text windows for education or tutorial data - divides display into 1st segment window for presentation of content related to selected menu category, and 2nd menu display segment for presentation of menu item and path data, tracing path to current display of content.
DC T01
IN LANE, M W; LANE, R S
PA (LANE-I) LANE M W; (LANE-I) LANE R S
CYC 1
PI US 5704051 A 19971230 (199807)* 8p G06F003-00 <--
ADT US 5704051 A Cont of US 1993-155464 19931119, US 1996-613527 19960311
PRAI US 1993-155464 19931119; US 1996-613527 19960311
IC ICM G06F003-00
AB US 5704051 A UPAB: 19980216
A data processor for managing a multilevel application wherein the data processor includes a display controller that creates a three-level menu window and a data window. The menu window includes two levels that each incorporate select commands associated with discrete subjects wherein menu commands are concurrently displayed on screen to provide historical access information.
Menu commands are converted into display presentations where each level defines a greater degree of information detail on a given subject. The data display window for these presentations is further divided into windows for text and graphics.
ADVANTAGE - Exceptionally effective at providing educational or tutorial information access in efficient manner.
Dwg.3/4
FS EPI
FA AB; GI
MC EPI: T01-J12B; T01-J12D

L72 ANSWER 2 OF 22 WPIX (C) 2003 THOMSON DERWENT
AN 1997-052594 [05] WPIX
DNN N1997-043087
TI Virtual environment creation, organisation and construction method in computer graphic - involves linking intermediate data files to create finished data files representing virtual environment, and completing new finished data file if geometry of object is altered.
DC T01
IN ALBERTSON, J; MCCOY, D S
PA (VIRT-N) VIRTUAL WORLD ENTERTAINMENT INC; (ALBE-I) ALBERTSON J; (MCCO-I) MCCOY D S
CYC 22
PI WO 9641313 A1 19961219 (199705)* EN 58p G06T011-40
RW: AT BE CH DE DK ES FI FR GB GR IE IT LU MC NL PT SE
W: AU CA JP MX
AU 9662723 A 19961230 (199716) G06T011-40
US 5710878 A 19980120 (199810) 22p G06T015-00 <--
ADT WO 9641313 A1 WO 1996-US10032 19960606; AU 9662723 A AU 1996-62723 19960606; US 5710878 A US 1995-480649 19950607
FDT AU 9662723 A Based on WO 9641313
PRAI US 1995-480649 19950607
REP 1.Jnl.Ref

IC ICM G06T011-40; G06T015-00
 AB WO 9641313 A UPAB: 19970129

The method involves collecting, managing and manipulating data during construction of a virtual environment, and automatically re-processing the sub-set of data necessary to produce a resource for use by a simulation program. The method provides for the repeated application of designated material to commonly designated elements of multiple objects (114). The method involves linking the intermediate data files to create the finished data files representing a virtual environment.

Once the material has been designated (110) to be applied to a particular element of an object (110), application to other objects is facilitated by designating the common element (102,104). If the geometry of an object or material is altered, the automated replication process completes the new finished data file.

USE - Collecting, managing, manipulating and checking data during construction of simulation environment including virtual environment, sound etc.

ADVANTAGE - Eliminates redundant manual processes using techniques to capture manipulations for later use. Minimises potential for error in data which would cause simulation program to crash or exhibit anomalies. Reduces amount of repetitive artist labour related to iterated operations performed, and improves error detection and indication.

Dwg.8/19

FS EPI
 FA AB; GI
 MC EPI: T01-J10C4A; T01-J40
 ABEQ US 5710878 A UPAB: 19980309

The method involves collecting, managing and manipulating data during construction of a virtual environment, and automatically re-processing the sub-set of data necessary to produce a resource for use by a simulation program. The method provides for the repeated application of designated material to commonly designated elements of multiple objects (114). The method involves linking the intermediate data files to create the finished data files representing a virtual environment.

Once the material has been designated (110) to be applied to a particular element of an object (110), application to other objects is facilitated by designating the common element (102,104). If the geometry of an object or material is altered, the automated replication process completes the new finished data file.

USE - Collecting, managing, manipulating and checking data during construction of simulation environment including virtual environment, sound etc.

ADVANTAGE - Eliminates redundant manual processes using techniques to capture manipulations for later use. Minimises potential for error in data which would cause simulation program to crash or exhibit anomalies. Reduces amount of repetitive artist labour related to iterated operations performed, and improves error detection and indication.

Dwg.11/19

L72 ANSWER 3 OF 22 WPIX (C) 2003 THOMSON DERWENT
 AN 1997-026220 [03] WPIX

DNN N1997-022014

TI Computer based interactive type three dimensional graphical system - controls graphical processing engine by supervisor controller to execute at least one graphical function using displayed command.

DC T01

IN BORREL, P; CHENG, K F; MENON, J P; ROSSIGNAC, J R
 PA (IBM) IBM CORP; (IBM) INT BUSINESS MACHINES CORP

CYC 3

PI JP 08287288 A 19961101 (199703)* 17p G06T015-00
 US 5708764 A 19980113 (199809) 18p G06T017-40 <--
 KR 246066 B1 20000315 (200122) G06T017-00

ADT JP 08287288 A JP 1996-34464 19960222; US 5708764 A Cont of US 1995-410370

19950324, US 1996-716816 19960910; KR 246066 B1 KR 1996-6246 19960309
 PRAI US 1995-410370 19950324; US 1996-716816 19960910
 IC ICM G06T015-00; G06T017-00; G06T017-40
 ICS G06T017-40

AB JP 08287288 A UPAB: 19970115

The system makes use of a processing engine and a supervisor controller. A graphical data continuing a three dimensional object is processed by the processing engine and is displayed in first part of a display table.

A text is displayed in the second part of the display table by user. The supervisor controller controls the processing engine to execute at least one graphical function with the displayed command.

ADVANTAGE - Enables to generate multiple side annotation windows effectively.

Dwg.2/10

FS EPI

FA AB; GI

MC EPI: T01-J10C4

ABEQ US 5708764 A UPAB: 19980302

The system makes use of a processing engine and a supervisor controller. A graphical data continuing a three dimensional object is processed by the processing engine and is displayed in first part of a display table.

A text is displayed in the second part of the display table by user. The supervisor controller controls the processing engine to execute at least one graphical function with the displayed command.

ADVANTAGE - Enables to generate multiple side annotation windows effectively.

Dwg.5/10

L72 ANSWER 4 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1996-485321 [48] WPIX

DNN N1996-408900

TI Synthesizing three dimensional multi-modality image sets into single composite image - extracting surfaces from two or more different images to be matched, and performing distance transformation for one surface image, and developing cost function for matching process using distance image.

DC S05 T01

IN JIANG, H; ROBB, R A

PA (MAYO-N) MAYO FOUNDATION

CYC 1

PI US 5568384 A 19961022 (199648)* 14p G06F159-00 <--

ADT US 5568384 A US 1992-960128 19921013

PRAI US 1992-960128 19921013

IC ICM G06F159-00

AB US 5568384 A UPAB: 19961202

The method involves extracting surfaces from two or more different images to be matched using semi-automatic segmentation techniques. The surfaces are represented as contours with common features to be matched. A distance transformation is performed for one surface image, and a cost function for the matching process is developed using the distance image. The geometric transformation includes three-dimensional translation, rotation and scaling to accommodate images of different position, orientation and size.

The matching process involves efficiently searching this multi-parameter space and adjusting a surface or surfaces to find the best fit among them which minimizes the cost function. The local minima problem is addressed by using a large number of starting points. A pyramid multi-resolution approach is employed to speed up both the distance transformation computation and the multi-parameter minimization processes.

USE/ADVANTAGE - Synthesizing base image data set and match image data set into single fused composite image data set with accurate registration and congruence, for e.g medical images i.e MR, PET and ultrasound imaging systems. Robustness in noise handling is accomplished using multiple thresholds embedded in the multi-resolution search. Enables registration of both partially overlapped and fragmented surfaces.

Dwg.8/8

FS EPI

FA AB; GI

MC EPI: S05-D02A5E; S05-D02B2; S05-D03E; T01-J06A; T01-J10C4

L72 ANSWER 5 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1994-255602 [31] WPIX

CR 1996-179576 [18]; 1997-384942 [35]; 2002-518157 [55]

DNN N1994-201282

TI Graphic data processing appts using displayed graphics for application program selection - has first storage device for storing number of data records each of which to basic display element displayed on display device.

DC T01

IN KITAGAWA, K; TANI, I

PA (KITA-I) KITAGAWA K; (TANI-I) TANI I; (DESI-N) DESIGN AUTOMATION INC; (OMRO) OMRON CORP

CYC 1

PI US 5337402 A 19940809 (199431)* 24p G06F005-62 <--

US 2002054147 A1 20020509 (200235) G06F013-00

ADT US 5337402 A Cont of US 1987-60910 19870612, CIP of US 1989-443832 19891201, US 1991-654182 19910213; US 2002054147 A1 Cont of US 1987-60910 19870612, CIP of US 1989-443832 19891201, Div ex US 1991-654182 19910213, Div ex US 1994-283894 19940803, Cont of US 1995-576375 19951221, Cont of US 1997-858809 19970519, US 1999-407069 19990928

PRAI JP 1986-137727 19860612

IC ICM G06F005-62; G06F013-00

AB US 5337402 A UPAB: 20020903

The appts uses a number of display elements for forming display device, first and second storage devices, a determining device for designating a basic display element of a portion of the display element displayed on the display device, a searching device for searching the first storage device for a data record corresp to the basic display element designated by the designating device, a selecting device for selecting drawing of either a basic display element or a composite display element constituting the display element displayed on the display device.

The appts also incorporates a program reading device for reading an application program for drawing the basic display element from the second storage device based on a first code of the data record searched for by the searching device in response to the selection of the basic display element by the selecting device.

USE/ADVANTAGE - In CAD/CAM systems. Provision for Quick and exact designation of commands to display graphic form, characters symbol etc on display screen.

Dwg.4/23

FS EPI

FA AB; GI

MC EPI: T01-J12B; T01-J15

L72 ANSWER 6 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1994-234155 [28] WPIX

CR 1997-020670 [02]; 1997-200962 [18]; 1998-239252 [21]

DNN N1994-185195 DNC C1994-106439

TI Prodn. of peptide or peptidomimetic drugs - by introducing chemically modified moieties based on conformation studies and testing for bio-activity.

DC B04 T01

IN BALAJI, V N; SINGH, C U

PA (BALA-I) BALAJI V N; (SING-I) SINGH C U

CYC 1

PI US 5331573 A 19940719 (199428)* 65p G06F015-42 <--

ADT US 5331573 A US 1990-628111 19901214

PRAI US 1990-628111 19901214

IC ICM G06F015-42

AB US 5331573 A UPAB: 19980528

Prodn. of a simulated, chemically modified peptide or peptidomimetic structures which mimic the energetically most probable 3-dimensional structure of preselected less constrained polypeptides, comprises (a) determining the phi and psi angles for each residue included in the preselected polypeptide, (b) comparing the phi and psi angles for each residue obtd. with the phi and psi angles for each residue of known polypeptide species, (c) substituting a chemically modified moiety for at least one of the residues of the preselected polypeptide to produce a chemically modified peptide or peptidomimetic structure, where the chemically modified moiety has phi and psi angles which are similar to the phi and psi angles of the residue that is replaced and (d) chemically synthesising and resting the bioactivity of the chemically modified peptide of peptidomimetic structure.

Also claimed is a method for generating biologically or pharmacologically active molecules comprising : (a) determining the amino acid sequence of the hypervariable region of a monoclonal antibody (MAb) having biological or pharmacological activity and (b) producing a peptidomimetic cpd. based on the amino acid sequence, where the peptidomimetic cpd. retains the biological or pharmacological activity of the MAb and the peptidomimetic cpd. is produced by: (i) determining the energetically most probable phi and psi angles for each residue included in the hypervariable region of the MAb, (ii) comparing the phi and psi angles for each residue obtd. in step (i) with the phi and psi angles for each residue of known polypeptide species and (iii) substituting a chemically modified moiety for at least one of the residues of the active cpd., where the chemically modified moiety has phi and psi angles which are similar to the phi and psi angles of the residue to be replaced.

ADVANTAGE - The methods provide for the rational design of cpds. which can be used as drugs. The obtd. drugs can have increased stability, e.g. increased metabolic stability, enhanced pharmacokinetic properties, e.g. increased absorption, distribution and/or elimination, enhanced potency, enhanced bioavailability, improved ease of synthesis and/or enhanced ease of administration.

Dwg.0/23

FS CPI EPI

FA AB; DCN

MC CPI: B04-C01; B04-N04

EPI: T01-J15A3

L72 ANSWER 7 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1994-191886 [23] WPIX

DNN N1994-150982 DNC C1994-087719

TI Chemical data handling system - includes display system for tabular form for many cpds. having chemical structures arranged along one axis and characteristic data along other axis.

DC B04 J04 T01

IN IMAMURA, F; KUSABA, S; MORI, K; YAMAMOTO, M; ARAI, M; TANIUCHI, K

PA (FUIT) FUJITSU LTD

CYC 1

PI US 5321804 A 19940614 (199423)* 29p G06F015-66 <--
US 37803 E 20020723 (200254) G06F015-00ADT US 5321804 A US 1991-725103 19910703; US 37803 E US 1991-725103 19910703,
US 1996-616225 19960315

FDT US 37803 E Reissue of US 5321804

PRAI JP 1990-179781 19900705; JP 1990-179782 19900705; JP 1990-179783
19900705; JP 1990-212809 19900810; JP 1990-248032 19900917

IC ICM G06F015-00; G06F015-66

AB US 5321804 A UPAB: 19940727

The chemical data handling system for editing and displaying compound data table consisting of chemical structure data and general data for compounds on a display screen, has a device for arranging the data of at least one

compound in the X-axis direction of the display screen. Chemical data for different compounds are arranged in the direction of axis Y crossing the X-axis direction of the display screen.

Data item names corresp. to the chemical structure and general data of the one compound are arranged along the X-axis, and a scrolling device scrolls a compound data table formed from the chemical structure and general data in the directions of both axes. The scroll device fixes data of a column displaying structures of compounds and shifts remaining general data columns in the direction of the axis X at the time of scrolling in the X-axis direction.

USE/ADVANTAGE - For graphical display of chemical analyses. Accommodates large amt. of data. Enables accurate copying of data between data tables.

Dwg.9/20

FS CPI EPI

FA AB

MC CPI: B11-C09; J04-C

EPI: T01-J10X

L72 ANSWER 8 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1993-287917 [36] WPIX

DNN N1993-221482 DNC C1993-128487

TI Computerised prediction of protein side-chain conformation - using steric interaction potential to rotate side-chains into low energy conformation which is identified.

DC B04 S03 T01

IN LEE, C; SUBBIAH, S

PA (STRD) UNIV LELAND STANFORD JUNIOR

CYC 1

PI US 5241470 A 19930831 (199336)*

23p G06F015-46 <--

ADT US 5241470 A US 1992-823790 19920121

PRAI US 1992-823790 19920121

IC ICM G06F015-46

AB US 5241470 A UPAB: 19931122

Method for determining the 3-D structure of a peptide (I), with aminoacid side chains extending from a defined main chain backbone, each aminoacid side chain having predefined rotational degrees of freedom, comprises (a) inputting coordinates of the main chain backbone of (I); (b) constructing an initla 3-D peptide conformation by placing the aminoacid side chains on the main chain backbone coordinates, (I) being in an initial 3-D peptide conformation; (c) randomly relating the aminoacid side chains around the predefined rotational degrees of freedom by small rotational perturbations to produce a modified 3-D peptide conformation; (d) determining the side chain steric interaction energy for the modified peptide conformation; and (e) creating a final 3-D peptide conformation by reducing the side chain steric interaction energy by repeating steps (c)-(d), where the step of randomly rotating is biased toward conformations having lower values of the side chain steric interaction energy and the interaction energy is truncated if it exceeds a preselected max.

USE - The method may be used to identify the packing configuration of mutant peptides.

Dwg.6c/7

FS CPI EPI

FA AB

MC CPI: B04-C01; B11-C08; B12-K04A

EPI: S03-E14H5; T01-J09

L72 ANSWER 9 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1993-045645 [05] WPIX

DNN N1993-034929 DNC C1993-020663

TI Characterising the three-dimensional structure of a protein - by analysing aminoacid residue positions and comparing with known protein structures.

DC B04 D16 T01

IN BOWIE, J U; EISENBERG, D; LUTHY, R
 PA (REGC) UNIV CALIFORNIA
 CYC 18

PI WO 9301484 A1 19930121 (199305)* EN 56p G06F015-20
 RW: AT BE CH DE DK ES FR GB GR IT LU MC NL SE
 W: AU CA JP

AU 9224082 A 19930211 (199321) G06F015-20
 US 5436850 A 19950725 (199535) 23p G06F019-00 <--
 ADT WO 9301484 A1 WO 1992-US5773 19920710; AU 9224082 A AU 1992-24082
 19920710; US 5436850 A Cont of US 1991-728640 19910711, US 1994-218685
 19940328

FDT AU 9224082 A Based on WO 9301484

PRAI US 1991-728640 19910711; US 1994-218685 19940328

REP US 4704692; US 4717653; US 4853871; US 4881175; US 4908773; US 4939666; US
 4946778; US 4976958; US 5087558

IC ICM G06F015-20; G06F019-00

ICS C12N015-00; C12Q001-68

AB WO 9301484 A UPAB: 19931119

Characterising the 3-dimensional(3-D) structure of a protein, comprises
 (a) determining, from the 3-D structure of the protein, values for a
 structural properties P1,P2....Pn for each amino acid residue position of
 the protein, (b) assigning each residue of the protein to one environment
 class based upon the values for the n structural properties P1,P2Pn
 for the residue, thereby generating a 1-dimensional environment string
 comprising the environment class of each residue in the 3-D protein
 structure.

USE/ADVANTAGE - Permit the assignment of many amino acid sequences to
 known 3-D structures. Used partic. for screening structural analogues of a
 known protein sequence. The 3-D compatibility searches are able to detect
 structural relationships that may not be apparent by sequence similarity.
 1/5

Dwg.1/5

FS CPI EPI

FA AB; GI

MC CPI: B04-B04A; B12-K04; D05-H09

EPI: T01-J10B2

ABEQ US 5436850 A UPAB: 19950905

The three-dimensional structure of a protein is characterised by
 determining values for n structural properties P1-Pn for each amino acid
 residue, and assigning each residue to one of a number of environmental
 classes based on the values to generate a one-dimensional environment
 string comprising the class of each residue. The data generated are input
 into a programmed computer which compares them to a database of other
 proteins of known structure and outputs analogous structures. The
 properties pref. include the total area of a residue side-chain buried by
 other protein atoms inaccessible to solvent, the fraction of the
 side-chain area covered by polar atoms or water, and the local secondary
 structure.

USE/ADVANTAGE - Partic. for identifying protein sequences which fold
 into a known three-dimensional structure. Relates a one-dimensional target
 sequence directly to known three-dimensional structures and effectively
 utilises information about the accommodation of sequence changes inherent
 in known structures.

Dwg.1/8

L72 ANSWER 10 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1992-373358 [45] WPIX

DNN N1992-284683

TI Apparatus for optical recognition of chemical graphics - allows documents
 contg. chemical structures to be optically scanned and converted directly
 into molecular structure files for direct input into chemical databases,
 molecular modelling programs etc..

DC T01 T04

IN BOYER, S K; CASEY, R G; MILLER, A M; OUDOT, B; ZILLES, K S
 PA (IBMC) INT BUSINESS MACHINES CORP

CYC 1

PI US 5157736 A 19921020 (199245)* 94p G06K009-00 <--

ADT US 5157736 A US 1991-688173 19910419

PRAI US 1991-688173 19910419

IC ICM G06K009-00

AB US 5157736 A UPAB: 19931006

The appts. includes separator for receiving a binary array of picture components representing a textual input which includes printed chemical structure indicia and for generating an isolated array of picture components representing the chemical structure. Vectorisation means responsive to the isolated array of picture components generates a vector representation of the printed chemical structure. Segmentation means responsive to the vector representation of separates character information from graphics information in the vector representation into sets of connected character vectors and sets of connected graphics vectors.

Vector clean up means responsive to the set sets of connected graphics vectors eliminate redundant vectors and vector junctions to generate optimised sets of connected graphics vectors. Optical character recogniser responsive to the sets of connected character vectors generates a character identification code corresp. to the sets of connected character vectors.

Graphical structure recogniser responsive to the optimised sets of graphics vectors for constructing an array of atoms and associated bond structure. Chemical formula recogniser automatically identifies chemical substrates in response to the character identification codes and generates chemical substructure connection tables with the array of atoms to generate a complete molecular structure file listing of atoms and associated bond structure.

ADVANTAGE - Saves time on creating graphical database. No duplication of work required often, as chemical structures that are candidates for addition to database, e.g. are often printed in journals, catalogues etc.

2/14

FS EPI

FA AB; GI

MC EPI: T01-J10A1; T01-J10B2; T04-D07C

L72 ANSWER 11 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1992-300238 [36] WPIX

CR 1994-366368 [45]

DNN N1992-229905

TI Technique for modelling the electron density of macromolecule - using multistep refining of data from correlation between calculated amplitudes and normalised values to calculate density.

DC S03 T01

IN SUBBIAH, S

PA (STRD) UNIV LELAND STANFORD JUNIOR

CYC 36

PI WO 9214211 A1 19920820 (199236)* EN 54p G06F015-00

RW: AT BE CH DE DK ES FR GB GR IT LU MC NL OA SE

W: AT AU BB BG BR CA CH CS DE DK ES FI GB HU JP KP KR LK LU MG MN MW
 NL NO PL RO RU SD SE US

AU 9213323 A 19920907 (199249) G06F015-00

US 5200910 A 19930406 (199316) 24p G06F015-20 <--

ADT WO 9214211 A1 WO 1992-US849 19920130; AU 9213323 A AU 1992-13323 19920130,
 WO 1992-US849 19920130; US 5200910 A US 1991-648788 19910130

FDT AU 9213323 A Based on WO 9214211

PRAI US 1991-648788 19910130

REP 2.Jnl.Ref; US 5025388; US 5103415

IC ICM G06F015-20

AB WO 9214211 A UPAB: 19950102

The method involves using a computer with an interface (33) to receive

data from a diffraction appts. (34), a memory unit (35) and file storage (36) e.g. magnetic disk or tape, and a CPU (37) to process the information. An output device (38) such as a printer or plotter provides a graphical display of electron density.

The technique comprises inputting experimental crystallographic data into a computer, distributing scattering bodies in a corresp. asymmetric unit and calculating scattering data. The correlation between experimental and calculated data is determined and thereafter at least one scatter is moved to enable a new distribution, new correlation and then a final distribution defining the electron density of the crystal, from the maximised repetitive steps to be made.

ADVANTAGE - Provides rapid determination of electron density of crystal without need to determine reflection phase.

1c/12

Dwg.1c/12

FS EPI

FA AB; GI

MC EPI: S03-E06C; T01-J07; T01-J15X

ABEQ US 5200910 A UPAB: 19931006

The method for modelling the electron density distribution of a macromolecule in a defined asymmetric unit of a crystal lattice involves producing an initial distribution of scattering bodies within a asymmetric unit having the same dimensions as the defined asymmetric unit. Scattering amplitudes of the initial distribution are calculated and the correlation between the calculated scattering amplitudes and the normalised amplitudes is determined. At least one of the scattering bodies is moved within the asymmetric unit to create a modified distributions. Scattering amplitudes and phases of the modified distribution are calculated and the correlation between the calculated amplitudes and the normalised values is determined. A final distribution of scattering bodies is produced by repeating moving and calculating steps until the correlation between the calculated scattering amplitudes and the normalised amplitudes is effectively maximised. The final distribution of scattering bodies defines the electron density of the crystal. ADVANTAGE - Simplified method to determine structure of crystalline molecules.

1c/12

L72 ANSWER 12 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1992-179147 [22] WPIX

DNC C1992-082137

TI Evaluation of configuration motif - is preformed using values obtd. from descriptive length of motif which express parts of the motif.

DC D16

IN KONAGAYA, A

PA (NIDE) NEC CORP

CYC 2

PI JP 04115360 A 19920416 (199222)* 9p G06F015-40

US 5410493 A 19950425 (199522) 14p G06F015-46

ADT JP 04115360 A JP 1990-236082 19900906; US 5410493 A US 1991-755364

19910906

PRAI JP 1990-236082 19900906

IC ICM G06F015-40; G06F015-46

ICA C12M001-00

AB JP 04115360 A UPAB: 19931006

Evaluation of a configuration motif is performed based on values calculated based on the descriptive length of a configuration motif expressing characteristic parts of a configuration and the descriptive length of the precision of the configuration motif.

USE - Prediction precision is improved.

0/0

FS CPI

FA AB

MC CPI: D05-H09

L72 ANSWER 13 OF 22 WPIX (C) 2003 THOMSON DERWENT
 AN 1991-340015 [46] WPIX
 DNN N1991-260465 DNC C1991-146838
 TI 3-dimensional protein structure determining method - processing full
 sequence of amino acid residues of protein using microprocessor for
 simulating folding of protein.
 DC J04 S03 T01
 IN SKOLNICK, J; KOLINSKI, A
 PA (SCRI) SCRIPPS CLINIC & RES FOUND; (SCRI-N) SCRIPPS CLINIC & RE
 CYC 20
 PI WO 9116683 A 19911031 (199146)*
 RW: AT BE CH DE DK ES FR GB GR IT LU NL SE
 W: AU CA FI JP NO
 AU 9178837 A 19911111 (199207)
 JP 05501324 W 19930311 (199315) 43p G06F015-20
 PT 97480 A 19930531 (199325) G06F007-00
 US 5265030 A 19931123 (199348) 74p G06F015-60
 ADT JP 05501324 W JP 1991-509821 19910423, WO 1991-US2786 19910423; PT 97480 A
 PT 1991-97480 19910424; US 5265030 A Cont of US 1990-513918 19900424, Cont
 of US 1991-803678 19911203, US 1992-932282 19920819
 FDT JP 05501324 W Based on WO 9116683
 PRAI US 1990-513918 19900424
 REP US 4704692; US 4853871; US 4881175; US 4908773; US 4939666; US 4985827
 IC ICM G06F007-00; G06F015-20; G06F015-60
 ICS G01N033-68; G06F015-42; G06F015-46
 AB WO 9116683 A UPAB: 19931220
 The method determines with a machine a three-dimensional structure of a
 protein or portion thereof including sidechains is claimed. A sequence of
 amino acid residues whose native tertiary structure is to be determined
 and local conformation preferences for respective residues of the sequence
 are specified.
 A temp. is also specified, and a representation of an unfolded chain
 of the residues in three dimensions is automatically generated. Folding of
 the chain and interactions between all pairs of sidechains are simulated,
 and the representation of the tertiary structure displayed.
 ADVANTAGE - Simulation of protein folding and prediction of tertiary
 structure are not only performed with greater success and accomplished
 faster than by many existing methods, but simulation itself becomes more
 manageable (tractable). @ (109pp Dwg.No.3/16)@
 FS CPI EPI
 FA AB; GI
 MC CPI: J04-C
 EPI: S03-E14H1; T01-J07
 ABEQ JP 05501324 W UPAB: 19930928
 Determining three-dimensional structure of protein or portion including
 side chains, using machine is claimed. Sequence of amino acid residues
 whose native tertiary structure is to be determined and local conformation
 preferences for respective residues of the sequence are specified.
 Temp. is also specified, and representation of unfolded chain of the
 residues in three dimensions is automatically generated. Folding of the
 chain and interactions between all pairs of side chains are simulated, and
 the representation of the tertiary structure displayed.
 ADVANTAGE - Simulation of protein folding and prediction of tertiary
 structure are not only performed with greater success and accomplished
 faster than by many existing methods, but simulation itself becomes more
 manageable (tractable)
 ABEQ US 5265030 A UPAB: 19940120
 Three-dimensional structures of globular proteins are determined by a
 computer-based system which is based on a Monte Carlo dynamics technique
 with asymmetric Metropolis sampling criterion. A sequence of amino acid
 residues of a protein is specified and a 210 lattice structure is created
 for each amino acid of the protein. An unfolded conformation consisting of

alpha-C backbone and side chains is represented spatially and successive likely tertiary conformations are selected, from which the lowest total-free-energy conformation is chosen. Coordinate set is created for display.

ADVANTAGE - Fast method of determining protein structures.
Dwg.15B/16

L72 ANSWER 14 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1991-324845 [44] WPIX

DNN N1991-249085

TI Transmitter location searching for multipath transmission environment - partitions monitored area into several cells and finds optima of total cost function at centres of cells.

DC W02 W06

IN HUANG, C C; PUCKETTE, C M

PA (GENE) GENERAL ELECTRIC CO

CYC 2

PI US 5058200 A 19911015 (199144)* <--

CA 2042275 A 19911205 (199209)

ADT US 5058200 A US 1990-533264 19900604

PRAI US 1990-533264 19900604

IC G01S003-04; H04B001-00; H04B007-00

AB US 5058200 A UPAB: 19930928

The transmitter location searching system in a multipath transmission environment geometrically partitions the monitored area into several cells and finds the optima of a total cost function at the centers of the cells. The original three-dimensional optimisation problem is reduced to a one-dimensional problem. Based on this calculation, the cell providing the smallest cost is chosen as a new candidate cell which is divided into smaller cells and the minimum costs are calculated for each of these smaller cells.

The cell provides the smallest cost is chosen as the center of another new candidate cell. The process is iterated until a dimension of a new candidate cell is smaller than a predetermined threshold. The dimensions of each cell is reduced by a factor of two at each iteration and the algorithm converges rapidly.

ADVANTAGE - Fast, stable and accurate results.

3/8

FS EPI

FA AB; GI

MC EPI: W02-C03C; W06-A02A

L72 ANSWER 15 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1991-200832 [27] WPIX

CR 1994-134991 [16]

DNN N1991-153609

TI Comparative molecular field analysis for 3D-QSAR - calculates steric and electrostatic interaction energies at spatial coordinates and uses partial least squares.

DC S03 S05 T01

IN CRAMER, R D; WOLD, S B; WOLD, S V; SVANTE, W

PA (TRIP-N) TRIPOS ASSOC INC; (CRAM-I) CRAMER R D; (WOLD-I) WOLD S; (SVAN-I) SVANTE W

CYC 16

PI US 5025388 A 19910618 (199127)* <--

WO 9222875 A1 19921223 (199302) # EN 54p G06F015-46

RW: AT BE CH DE DK ES FR GB GR IT LU NL SE

W: DE GB JP

GB 2266391 A 19931027 (199342) # 1p G06F015-46

EP 592421 A1 19940420 (199416) # EN 2p G06F015-46

R: AT BE CH DE DK ES FR GB IT LI NL SE

JP 06503908 W 19940428 (199422) # G06F015-20

EP 592421 A4 19940831 (199533)

EP 592421 B1 19970326 (199717) EN 34p G06F017-17
 R: AT BE CH DE DK ES FR GB IT LI NL SE
 DE 69125399 E 19970430 (199723)# G06F017-17
 ADT US 5025388 A US 1988-237491 19880826; WO 9222875 A1 WO 1991-US4292
 19910617; GB 2266391 A WO 1991-US4292 19910617, GB 1993-15049 19930720; EP
 592421 A1 EP 1991-913619 19910617, WO 1991-US4292 19910617; JP 06503908 W
 JP 1991-512615 19910617, WO 1991-US4292 19910617; EP 592421 A4 EP
 1991-913619 ; EP 592421 B1 EP 1991-913619 19910617, WO 1991-US4292
 19910617; DE 69125399 E DE 1991-625399 19910617, EP 1991-913619 19910617,
 WO 1991-US4292 19910617
 FDT GB 2266391 A Based on WO 9222875; EP 592421 A1 Based on WO 9222875; JP
 06503908 W Based on WO 9222875; EP 592421 B1 Based on WO 9222875; DE
 69125399 E Based on EP 592421, Based on WO 9222875
 PRAI US 1988-237491 19880826; WO 1991-US4292 19910617; GB 1993-15049
 19930720; EP 1991-913619 19910617; JP 1991-512615 19910617; DE
 1991-625399 19910617
 REP US 4461619; US 4473889; US 4642762; US 5025388; 2.Jnl.Ref; EP 431189; WO
 9104543; EP 436597; US 4473890
 IC ICM G06F015-20; G06F015-46; G06F017-17
 ICS G06F013-46; G06F017-50
 ICI G06F159-00, G06T017:
 AB US 5025388 A UPAB: 19970424

Comparative Molecular Field Analysis (CoMFA) is an effective computer implemented methodology of 3D-QSAR employing both interactive graphics and statistical techniques for correlating shapes of molecules with their observed biological properties. For each molecule of a series of known substrates the steric and electrostatic interaction energies with a test probe atom are calculated at spatial coordinates around the molecule. Subsequent analysis of the data table by a partial least squares (PLS) cross-validation technique yields a set of coefficients which reflect the relative contribution of the shape elements of the molecular series to differences in biological activities.

Display in three dimensions in an interactive graphics environment of the spatial volumes highly associated with biological activity, and comparison with molecular structures yields an understanding of intermolecular associations. CoMFA will also predict the biological activity of new molecular species.

USE - For understanding structure/function relationships in biological chemistry. @(21pp Dwg.No.2/5)@

FS EPI
 FA AB; GI
 MC EPI: S03-E14H; S05-C09; T01-J07; T01-J10B
 ABEQ GB 2266391 A UPAB: 19931202

Comparative Molecular Field Analysis (CoMFA) is an effective computer implemented methodology of 3D-QSAR employing both interactive graphics and statistical techniques for correlating shapes of molecules with their observed biological properties. For each molecule of a series of known substrates the steric and electrostatic interaction energies with a test probe atom are calculated at spatial coordinates around the molecule. Subsequent analysis of the data table by a partial least squares (PLS) cross-validation technique yields a set of coefficients which reflect the relative contribution of the shape elements of the molecular series to differences in biological activities.

Display in three dimensions in an interactive graphics environment of the spatial volumes highly associated with biological activity, and comparison with molecular structures yields an understanding of intermolecular associations. CoMFA will also predict the biological activity of new molecular species.

USE - For understanding structure/function relationships in biological chemistry. @(21pp Dwg.No.2/5)@
 Dwg.1/1

ABEQ EP 592421 B UPAB: 19970424
 Comparative Molecular Field Analysis (CoMFA) is an effective computer

implemented methodology of 3D-QSAR employing both interactive graphics and statistical techniques for correlating shapes of molecules with their observed biological properties. For each molecule of a series of known substrates the steric and electrostatic interaction energies with a test probe atom are calculated at spatial coordinates around the molecule. Subsequent analysis of the data table by a partial least squares (PLS) cross-validation technique yields a set of coefficients which reflect the relative contribution of the shape elements of the molecular series to differences in biological activities.

Display in three dimensions in an interactive graphics environment of the spatial volumes highly associated with biological activity, and comparison with molecular structures yields an understanding of intermolecular associations. CoMFA will also predict the biological activity of new molecular species.

USE - For understanding structure/function relationships in biological chemistry.
Dwg.1/9

L72 ANSWER 16 OF 22 WPIX (C) 2003 THOMSON DERWENT
AN 1991-095848 [14] WPIX
DNN N1991-074096
TI Data base information retrieval system - uses ordered identifiers to access information from sequential file such that only retrieval objects with high query scores are accessed.
DC T01
IN MITSUI, K
PA (IBMC) IBM CORP; (IBMC) INT BUSINESS MACHINES CORP
CYC 4
PI EP 420424 A 19910403 (199114)* 14p
R: DE FR GB
EP 420424 A3 19921202 (199343) 14p
US 5263159 A 19931116 (199347) 12p G06F015-40 <--
EP 420424 B1 19971203 (199802) EN 16p G06F017-30
R: DE FR GB
DE 69031772 E 19980115 (199808) G06F017-30
ADT EP 420424 A EP 1990-309707 19900905; EP 420424 A3 EP 1990-309707 19900905;
US 5263159 A US 1990-584305 19900918; EP 420424 B1 EP 1990-309707 19900905; DE 69031772 E DE 1990-631772 19900905, EP 1990-309707 19900905
FDT DE 69031772 E Based on EP 420424
PRAI JP 1989-242421 19890920
REP NoSR.Pub; 1.Jnl.Ref; DE 3901485; US 4358824
IC G06F015-40
ICM G06F015-40; G06F017-30
AB EP 420424 A UPAB: 19931207
The system includes two files in external storage: a sequential file (15) where data related to a retrievable object is identified and outputted; a transposed file (11) containing data and identifiers related to objects that include a specified key and are outputted when the key is selected. A query input technique is included that requires a combination of specified access keys with given weighting functions and a number n specifying the number of objects to be outputted.
An information retrieval method responds to the input query, accesses the transposed file and copies selected data into the main storage. A query score is computed for each object and the highest score is determined for the n objects. The sequential file is accessed using the identifiers of the objects with the highest score. @(14pp Dwg.No.3/5)@+
3/5
FS EPI
FA AB; GI
MC EPI: T01-J05B
ABEQ US 5263159 A UPAB: 19940111
What is claimed is:
The information retrieval method involves selecting, using the

processor, an access key in the query having the highest weighting coefficient which has not been previously selected, responsive to the inputting of a query. Next, copying data into the main memory from the transposed file which contains the retrieval object identifiers which are associated with the selected access key. Then, calculating, using the processor, for each retrieval object identifier a cumulative query score by adding the weighting coefficient for the selected access key to a previously calculated cumulative query score, if any, for each retrieval object which contains the selected access key.

The method also involves determining, using the processor, for each retrieval object a maximum anticipated score by adding the weighting coefficient for all access keys not previously selected to a previously calculated cumulative query score, if any, for each retrieval object identifier. Then, ranking, using the processor, the cumulative query scores for retrieval object identifiers from highest to lowest to create a rank list. Next, repeating the selecting, copying, calculating, determining and ranking steps until all access keys in the query have been selected or the cumulative query score at the N-th element in the rank list exceeds the maximum anticipated score for any retrieval object with a cumulative query score at the (N+1)-th element in the rank list or below. N retrieval objects are read corresponding to the N retrieval object identifiers having the highest cumulative query scores from the sequential file into the main memory.

USE/ADVANTAGE - for computerised quantitative data retrieval.
Effective way to reduce frequency of access to external file.
Dwg.1/5

ABEQ EP 420424 A UPAB: 19931207

The system includes two files in external storage: a sequential file (15) where data related to a retrievable object is identified and outputted; a transposed file (11) containing data and identifiers related to objects that include a specified key and are outputted when the key is selected. A query input technique is included that requires a combination of specified access keys with given weighting functions and a number n specifying the number of objects to be outputted.

An information retrieval method responds to the input query, accesses the transposed file and copies selected data into the main storage. A query score is computed for each object and the highest score is determined for the n objects. The sequential file is accessed using the identifiers of the objects with the highest score. @ (14pp Dwg.No.3/5)@+

ABEQ EP 420424 B UPAB: 19980112

The system includes two files in external storage: a sequential file (15) where data related to a retrievable object is identified and outputted; a transposed file (11) containing data and identifiers related to objects that include a specified key and are outputted when the key is selected. A query input technique is included that requires a combination of specified access keys with given weighting functions and a number n specifying the number of objects to be outputted.

An information retrieval method responds to the input query, accesses the transposed file and copies selected data into the main storage. A query score is computed for each object and the highest score is determined for the n objects. The sequential file is accessed using the identifiers of the objects with the highest score.
Dwg.1/5

L72 ANSWER 17 OF 22 WPIX (C) 2003 THOMSON DERWENT
AN 1991-022356 [03] WPIX

DNN N1991-017148

TI Measuring position and posture of object - obtaining projection points by moving camera to find line of points on intersection between planes and reference line.

DC S02 T01 T04 X25

IN KAWAKAMI, S; MORITA, T

PA (FUITS) FUJITSU LTD

CYC 7

PI WO 9016037 A 19901227 (199103)* 114p

RW: DE FR GB

W: AU CA JP US

AU 9058352 A 19910108 (199116)

EP 431191 A 19910612 (199124)

R: DE FR GB

JP 02509055 X 19910606 (199129)

EP 431191 A4 19940112 (199528)

US 5446798 A 19950829 (199540)

CA 2035034 C 19980120 (199816)

EP 431191 B1 19990901 (199940) EN

71p G06K009-00

<--

G06T009-20

G01B011-00

R: DE FR GB

DE 69033269 E 19991007 (199947)

G01B011-00

ADT EP 431191 A EP 1990-909392 19900620; JP 02509055 X JP 1990-311 19900620;

EP 431191 A4 EP 1990-909392 ; US 5446798 A Cont of WO 1990-JP811

19900620, Cont of US 1991-655373 19910220, Cont of US 1992-929505

19920818, US 1994-201082 19940224; CA 2035034 C CA 1990-2035034 19900620;

EP 431191 B1 EP 1990-909392 19900620, WO 1990-JP811 19900620; DE 69033269

E DE 1990-633269 19900620, EP 1990-909392 19900620, WO 1990-JP811 19900620

FDT EP 431191 B1 Based on WO 9016037; DE 69033269 E Based on EP 431191, Based on WO 9016037

PRAI JP 1989-157906 19890620; JP 1990-311 19900620

REP JP 59184973; JP 63113782; JP 64021305; 1.Jnl.Ref

IC G01B011-00; G06F015-62

ICM G01B011-00; G06K009-00; G06T009-20

ICS G01B011-26; G06F015-62; G06T007-00

AB WO 9016037 A UPAB: 19991122

Projection points are determined for various camera positions by moving the camera in a predetermined direction in order to determine a line of moving points on the intersection between a plane containing the predetermined centres of projection corresponding to the camera positions and the predetermined plane. A line of reference points arranged on the intersection between one plane passing through the centres of projection and the plane sharing one point with the line of moving points and having an equal cross ratio is prepared.

Each point on the line of moving reference points that correspond to each other are connected by the intersection between the plane containing corresponding points and the predetermined centres of projection and the predetermined plane. The points of intersection of these intersections is obtained and geometric data relating to the graphic elements of the object of measurement with reference to the camera positions in a three-dimensional space are obtained on the basis of the positions of the point of intersection.

USE - Image processing.

Dwg.16/42

FS EPI

FA AB; GI

MC EPI: S02-A03B4; S02-A09; T01-J10; T04-D02; X25-A03E

ABEQ US 5446798 A UPAB: 19951011

The method involves using a camera and moving it in a predetermined direction w.r.t. an object subject to measurement. Images of the object are taken at a number of camera positions from which contour images are respectively extracted. Image elements in each image are projected onto a point on a predetermined projection surface from a predetermined projection centre corresponding to a camera centre. Projected points are then obtained on the predetermined projection surface as a sequence of movement points ($x_t, t=0, 1, 2, \dots$) which line up on an intersection line.

Points which line up on a second intersection line are generated as a sequence of reference points ($t_{aut}, t=0, 1, 2, \dots$). A second plane containing the projection centre is also generated so that the sequences of reference and movement points share a point. An initial intersection point of further intersection lines is obtained at which respective planes

intersect the projection surface. The planes each contain the projection centre and a single movement and reference point from each respective sequence. Geometrical information is then obtained on the object w.r.t the camera position.

USE/ADVANTAGE - For providing three-dimensional information to robot. Functions stably in environment having complicated scenery.
Dwg.12/42

L72 ANSWER 18 OF 22 WPIX (C) 2003 THOMSON DERWENT
AN 1990-030146 [04] WPIX
CR 1987-327750 [46]
DNN N1990-023122 DNC C1990-013118
TI Computer based method useful in design of single chain proteins - determining and displaying structures for converting double-or multiple-chain polypeptides to single-chain.
DC B04 D16 J04 S03 S05 T01
IN LADNER, R C
PA (GENE) GENERAL ELECTRIC CO
CYC 1
PI US 4881175 A 19891114 (199004)* 34p <--
ADT US 4881175 A US 1988-204940 19880609
PRAI US 1986-902970 19860902; US 1987-115919 19871102; US 1988-204940 19880609
IC G01N033-00; G06F015-46
AB US 4881175 A UPAB: 19950425
The method determines and displays possible chemical structures for converting two naturally aggregated but chemically separated polypeptide chains into a single polypeptide chain which will fold into a three dimensional structure very similar to the original structure made of the two polypeptide chains.
A data base contains a large number of amino acid sequences for which the three dimensional structure is known. After plausible sits have been selected, this data base is examined to find which amino acid plausible sites to create a plausible one-polypeptide structure. The span (a scaler quantity) of the candidate is compared to the span of the gap. If the span is close enough, step two is done which involves aligning the first peptides of the candidate with the initial peptide of the gap.
1/20
Dwg.1/20
FS CPI EPI
FA AB; GI
MC CPI: B04-C01; B11-C09; B12-K04E; D05-H09; J04-B
EPI: S03-E14H; S05-C; T01-J09

L72 ANSWER 19 OF 22 WPIX (C) 2003 THOMSON DERWENT
AN 1989-280747 [39] WPIX
DNN N1989-214312 DNC C1989-124145
TI Consecutive forming method of high molecular cpd. - in which maps of portions to be determined in advance are formed in formats contg. information corresp. to X-Y-Z coordinate of polypeptide p.
DC B04 D16
PA (GEMX) GENEX CORP
CYC 2
PI JP 01158574 A 19890621 (198939)* 53p
US 4939666 A 19900703 (199029) <--
ADT JP 01158574 A JP 1988-221223 19880902; US 4939666 A US 1987-92147 19870902
PRAI US 1987-92147 19870902
IC C07B061-00; C07K003-00; C12N015-00; C12P021-02; G06F003-14; G06F015-60
AB JP 01158574 A UPAB: 19930923
In forming high molecular cpds. in a consecutive computerised manner for modifying structures contg. polypeptide portions to be determd. practically in advance with previously determd. conformations. Maps of portions to be determd. in advance are formed in formats contg.

information corresp. to the X-Y-Z coordinate of polypeptide portion to be determd. in advance and also information corresp. to local nonspacial characteristics in the first step(a). Aminoacid residual gps. to be added to existing structure are specified in a consecutively increased manner, and selected for conformance with the additional characteristics of the locality by testing lapped oligopeptide blocks in the second step(b), and polypeptide chains corresp. to several polypeptide portions of structures to be determd. practically in advance which corresp. to the structures to be specified in the step(b) and also given in at least the step(a) are synthesised in the third step(c).

USE/ADVANTAGE - Forms high molecular cpds. having structures which exist not always in natural field, e.g. proteins etc. including antibody, etc., in an artificial and computerised method. (Provisional Basic previously advised in week 8931).

0/5

FS CPI

FA AB

MC CPI: B04-B04A; B04-B04C; B04-C01; D05-C

ABEQ US 4939666 A UPAB: 19930923

Computer-assisted method modified a structure using 2 or more blocks between a starting point and an end point. Process comprises (a) mapping a first block onto starting point to produce information xyz coordinates and 1 or more non-spatial parameter of this block, (b) incrementally adding a second block to first block or to end point by mapping to produce information including xyz coordinates and 1 or more non-spatial parameter of second block, and (c) synthesising structure with each block.

USE - For constructing a polypeptide chain of predetermined conformation.

L72 ANSWER 20 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1989-055618 [08] WPIX

DNN N1989-042361

TI Query-words-sequence-content matching library document retrieval - locating target sequences of words and computing similarity values as function of corresponding equivalence values.

DC T01

IN BARBIC, F; CHOY, D M H; CHOY, D M

PA (IBMC) IBM CORP; (IBMC) INT BUSINESS MACHINES CORP

CYC 4

PI EP 304191 A 19890222 (198908)* EN 14p

R: DE FR GB

US 4823306 A 19890418 (198918) 10p

EP 304191 A3 19920527 (199331)

EP 304191 B1 19951213 (199603) EN 17p G06F017-30

R: DE FR GB

DE 3854774 G 19960125 (199609)

G06F017-30

ADT EP 304191 A EP 1988-307160 19880803; US 4823306 A US 1987-85110 19870814; EP 304191 A3 EP 1988-307160 19880803; EP 304191 B1 EP 1988-307160 19880803; DE 3854774 G DE 1988-3854774 19880803, EP 1988-307160 19880803

FDT DE 3854774 G Based on EP 304191

PRAI US 1987-85110 19870814

REP No-SR.Pub; 2.Jnl.Ref; EP 75903; 02Jnl.Ref

IC G06F015-40

ICM G06F017-30

ICS G06F015-40

AB EP 304191 A UPAB: 19931118

The method includes the steps of defining a set of equivalent words for each of the query words and assigning a word equivalence value to each of the equivalent words. Then, computing a relevance factor for a library document by locating target sequences of words in the library document that match the sequence of query words and equivalence, according to a set of matching criteria.

The similarity values of the target sequences of words are evaluated

as a function of the equivalence values of words included in the corresponding target sequence. The relevance factor is computed as a function of the similarity values of its target sequences.

USE/ADVANTAGE - For data processing system. High accuracy and flexibility.

1/1

FS EPI

FA AB; GI

MC EPI: T01-E01; T01-J05B

ABEQ US 4823306 A UPAB: 19930923

The method includes the steps of defining a set of equivalent words for each query word and assigning to each equivalent word a corresponding word equivalence value and locating target sequences of words in a library document that match the sequence of query words in accordance with a set of matching criteria.

A similarity is evaluated for each of target sequences words as a function of the corresponding equivalence values of words and a relevance factor is obtained for the library document based upon the similarity values of its target sequences.

ADVANTAGE - Higher accuracy and flexibility.

ABEQ EP 304191 B UPAB: 19960122

A method implemented in data processing apparatus for facilitating the retrieval from among more than one library document those matching the content of a sequence of query words, comprising the steps of:

(a) defining a set of equivalent words for each of the query words and assigning a word equivalence value (Sjk) to each of said equivalent words; and

(b) computing a relevance factor for one or more library documents, by the steps of:

(i) locating library documents that include one or more of the query words, and equivalents thereof;

(ii) evaluating similarity values (Sxyz) for said located library documents, each similarity value (Sxyz) being evaluated as a function of the equivalence values (Sjk) of words included in the library document, said relevance factor being computed as a function of the similarity values; and

(c) ranking the library documents in order of their respective relevance factors,

characterised in that the similarity values (Sxyz) are evaluated using matching algorithms (Axyz) for matching sequence of words in the located library documents to the sequence of query words, the function of the equivalence values including one or more weighting factors (d(fxz), g(xz)) based upon positions (fxz) of words in the located library documents.

Dwg.1/1

L72 ANSWER 21 OF 22 WPIX (C) 2003 THOMSON DERWENT

AN 1988-307666 [43] WPIX

DNN N1988-233421 DNC C1988-136113

TI Computer based method for protein engineering - by identifying sites which could be converted to cysteine residues to create stabilising di sulphide bond.

DC D16 D25 J04

IN LADNER, R C; PANTOLIANO, M W

PA (GEMX) GENEX CORP

CYC 13

PI WO 8808165 A 19881020 (198843)* EN 77p

RW: AT BE CH DE FR GB IT LU NL SE

W: DK JP

US 4853871 A 19890801 (198938) 23p

ADT WO 8808165 A WO 1988-US850 19880318; US 4853871 A US 1987-34966 19870406 <--

PRAI US 1987-34966 19870406

REP US 4704692; US 4719582

IC G01N033-00; G06F015-46
 AB WO 8808165 A UPAB: 19930923

The computer based method evaluates a protein's structure to determine whether the protein contains at least 2 target amino acid residues, the replacement of at least one of which with a cysteine residue would be sufficient to permit the formation of at least one potentially protein-stabilising disulphide bridge. The method comprises (a) examining each selected pair of amino acid residues in the protein to determine if they contain certain atoms whose relative 3-dimensional positions possess a geometric conformation similar to the corresp. atoms of a known disulphide bridge, (b) examining any pair of amino acids found to contain the certain atoms identified in (a) to determine whether the new atoms of a possible disulphide linkage can be accommodated without creating unacceptable steric hindrance, (c) permitting an expert operator (i) to view any possible sites for novel disulphide linkage which can be accommodated without altering the tertiary conformation of the protein molecule and (ii) to rank the viewed possible sites for a novel disulphide linkage from most likely to stabilise an engineered protein, to least likely to stabilise the protein and (d) evaluating the ranked possible sites for a novel disulphide linkage according to expert rule criterion.

USE/ADVANTAGE - The computer based method is used for selecting sites in natural proteins where the introduction of a novel disulphide linkage will have a high probability for stabilising a particular protein. The method may be applied to the modification of subtilisin (see example) which may be used in fabric washing compsns. contg. detergents.

0/8
 FS CPI
 FA AB
 MC CPI: D05-A02C; D11-B02; J04-C03
 ABEQ US 4853871 A UPAB: 19930923

Computer-based evaluation of protein structure determines whether it has 2 or more target amino acid residues, replacement of 1 or more with a cysteine residue permitting formation of 1 or more potentially protein-stabilising disulphide bonds.

Process comprises (a) examining each pair of residues in protein to see if they contain atoms whose 3-dimensional positions have a geometric conformation similar to those of disulphide bonds; (b) examining pairs of amino acids found to contain such atoms to see whether disulphide bond can be accommodated without creating unacceptable steric hindrance; (c) permitting an expert operator to view such a bond and rank it from: most likely to stabilise an engineered protein to one least likely to stabilise protein; and (d) evaluating ranked bond wrt expert rule criterion.

ADVANTAGE - Engineereed proteins can be produced by manipulating DNA sequences encoding them by incorporation into a plasmid.

L72 ANSWER 22 OF 22 WPIX (C) 2003 THOMSON DERWENT
 AN 1988-161435 [23] WPIX
 DNN N1988-123285 DNC C1988-072011

TI Computer method and system for naming chemical cpds. - by reducing structural data to components, naming these and constructing a connection table.

DC J04 T01 U21
 IN HIRYAMA, K; TIAZO, T
 PA (SUNR) SUNTORY LTD

CYC 1

PI US 4747059 A 19880524 (198823)* 35p <--
 ADT US 4747059 A US 1985-809514 19851216

PRAI US 1984-681688 19841214; US 1985-809514 19851216

IC G06F003-14; G06F015-20

AB US 4747059 A UPAB: 19930923

Naming chemical cpds. comprises (1) pre-setting name stems and 3 rules into computer memory; (2) inputting data representing the cpd.; (3) breaking the data down into components, each representing a constituent

element; (4) identifying a first data component (DC) using the first rule; (5) naming first DC according to the second rule; (6) constructing a connection table based on first DC and storing this in memory; (7) naming a second DC according to the third rule; (8) modifying the connection table by adding the name of the second DC; (9) repeating the process for all further DC and (10) determining and displaying the name of the cpd. on the basis of the final connection table. Also new is an appts. for the process.

USE/ADVANTAGE - The method is particularly applied to organic cpds. (including novel cpds.) and allows them to be named simply and without ambiguity. A natural language is used formula notation so is suitable for visual or aural display.

1/2

FS CPI EPI
FA AB; GI
MC CPI: J04-B
EPI: T01-J09; U21-A05D1

=> fil medline

FILE 'MEDLINE' ENTERED AT 10:20:10 ON 06 MAY 2003

FILE LAST UPDATED: 3 MAY 2003 (20030503/UP). FILE COVERS 1958 TO DATE.

On April 13, 2003, MEDLINE was reloaded. See HELP RLOAD for details.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2003 vocabulary. See <http://www.nlm.nih.gov/mesh/changes2003.html> for a description on changes.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all tot

L81 ANSWER 1 OF 3 MEDLINE
AN 95345057 MEDLINE
DN 95345057 PubMed ID: 7619787
TI **MolView:** a program for analyzing and displaying atomic structures on the Macintosh personal computer.
AU **Smith T J**
CS Department of Biological Sciences, Purdue University, West Lafayette, Indiana 47907, USA.
SO JOURNAL OF MOLECULAR GRAPHICS, (1995 Apr) 13 (2) 122-5, 115.
CY Journal code: 9014762. ISSN: 0263-7855.
DT United States
LA Journal; Article; (JOURNAL ARTICLE)
FS English
EM Priority Journals
ED 199508
Entered STN: 19950911
Last Updated on STN: 19950911
Entered Medline: 19950831
AB A program is described that allows the user to analyze and display atomic structures on any Macintosh personal computer. The program reads ASCII format structure files including PDB, plot files from the graphics programs O and FRODO, and Cartesian coordinates from ChemDraw 3D. The program has a graphical interface that features floating button palettes for objects and tools. The structures may be displayed using stick, ball-and-stick, space-filling, and ribbon models. Each type of drawing can be colored according to a variety of schemes to accentuate various structural aspects. The figures can be rotated, displayed in stereo, and exported using the Clipboard, PICT files, or Quick-Time movies. The

structure can be further analyzed by displaying hydrogen bonds, making Ramachandran plots, labeling atoms, measuring distances, and finding neighboring atoms. By using the Macintosh computer and emphasizing a graphical interface, this program helps to bring structural analysis to students and researchers that may not have access to, or experience with, large graphics workstations. In addition, the object-oriented output PICT images are ideal for creating publication-ready diagrams that can be easily modified or inserted into other documents (e.g., see Refs. 1-3).

CT *Computer Graphics
Man-Machine Systems
Microcomputers
*Models, Molecular
*Molecular Structure
Software Design

L81 ANSWER 2 OF 3 MEDLINE
AN 93028351 MEDLINE
DN 93028351 PubMed ID: 1409565
TI Fast structure alignment for protein databank searching.
AU Orengo C A; Brown N P; Taylor W R
CS National Institute for Medical Research, London, England.
SO **PROTEINS**, (1992 Oct) 14 (2) 139-67.
Journal code: 8700181. ISSN: 0887-3585.

CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199210
ED Entered STN: 19930122
Last Updated on STN: 19930122
Entered Medline: 19921029

AB A fast method is described for searching and analyzing the protein structure databank. It uses secondary structure followed by residue matching to compare protein structures and is developed from a previous structural alignment method based on dynamic programming. Linear representations of secondary structures are derived and their features compared to identify equivalent elements in two proteins. The secondary structure alignment then constrains the residue alignment, which compares only residues within aligned secondary structures and with similar buried areas and torsional angles. The initial secondary structure alignment improves accuracy and provides a means of filtering out unrelated proteins before the slower residue alignment stage. It is possible to search or sort the protein structure databank very quickly using just secondary structure comparisons. A search through 720 structures with a probe protein of 10 secondary structures required 1.7 CPU hours on a Sun 4/280. Alternatively, combined secondary structure and residue alignments, with a cutoff on the secondary structure score to remove pairs of unrelated proteins from further analysis, took 10.1 CPU hours. The method was applied in searches on different classes of proteins and to cluster a subset of the databank into structurally related groups. Relationships were consistent with known families of protein structure.

CT Check Tags: Animal; Comparative Study; Human
Amino Acid Sequence
*Databases, Factual
*Information Storage and Retrieval
Molecular Sequence Data
*Protein Structure, Secondary
Reference Standards
*Sequence Alignment
Sequence Homology, Amino Acid
Software
Time Factors

L81 ANSWER 3 OF 3 MEDLINE
AN 92260537 MEDLINE
DN 92260537 PubMed ID: 1583693
TI Common spatial arrangements of backbone fragments in homologous and non-homologous proteins.
AU **Alexandrov N N**; Takahashi K; Go N
CS Department of Chemistry, Faculty of Science, Kyoto University, Japan.
SO JOURNAL OF MOLECULAR BIOLOGY, (1992 May 5) 225 (1) 5-9.
Journal code: 2985088R. ISSN: 0022-2836.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Priority Journals
EM 199206
ED Entered STN: 19920626
Last Updated on STN: 20000303
Entered Medline: 19920616
AB We have developed a new method of detecting common spatial arrangements of backbone fragments in proteins. This method allows corresponding fragments to occur in a different order in respective amino acid sequences. We applied this method to detect structural similarities between an acid protease, endothiapepsin, and all other proteins in the protein data bank. Significant similarities were found not only with other acid proteases but also with virus proteases and with proteins having different functions. The possible biological meaning of these similarities is discussed.
CT Check Tags: Support, Non-U.S. Gov't
Aspartic Endopeptidases: CH, chemistry
Aspartic Endopeptidases: ME, metabolism
Databases, Factual
Models, Molecular
*Peptide Fragments: CH, chemistry
*Protein Conformation
Sequence Homology, Nucleic Acid
Software
Spectrum Analysis, Raman
CN 0 (Peptide Fragments); EC 3.4.23 (Aspartic Endopeptidases); EC 3.4.23.- (Endothia aspartic proteinase)

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FILE COVERS 1907 - 6 May 2003 VOL 138 ISS 19
FILE LAST UPDATED: 5 May 2003 (20030505/ED)

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=> d all 183

L83 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS
AN 1992:55008 HCAPLUS
DN 116:55008
TI Detection of common three-dimensional substructures in proteins
AU **Vriend, Gerrit**; Sander, Chris
CS Eur. Mol. Biol. Lab., Heidelberg, D-6900, Germany
SO Proteins: Structure, Function, and Genetics (1991), 11(1),
52-8
CODEN: PSFGEY; ISSN: 0887-3585
DT Journal
LA English
CC 9-16 (Biochemical Methods)
Section cross-reference(s): 6
AB A fully automatic algorithm is presented for 3-dimensional alignment of
protein structures and for the detection of common substructures and
structural repeats. Given 2 proteins, the algorithm first identifies all
pairs of structurally similar fragments and subsequently clusters into
larger units pairs of fragments that are compatible in 3 dimensions. The
detection of similar substructures is independent of insertion/deletion
penalties and can be chosen to be independent of the topol. of loop
connections and to allow for reversal of chain direction. By using
distance geometry filters and other approxns., the algorithm, implemented
in the WHAT IF program, is so fast that structural comparison of a single
protein with the entire database of known protein structures can be
performed routinely on a workstation. The method reproduces known
nontrivial superpositions such as plastocyanin on azurin. In addn. the
surprising structural similarity between ubiquitin and a (2Fe-2S)
ferredoxin is reported.
ST three dimensional substructure protein algorithm
IT Ferredoxins
RL: ANST (Analytical study)
(2-iron-2-sulfur, 3-dimensional substructures in, algorithm for study
of)
IT Azurins (proteins)
Hemoglobins
Plastocyanins
RL: ANST (Analytical study)
(3-dimensional substructures in, algorithm for study of)
IT Proteins, properties
RL: PRP (Properties)
(common 3-dimensional substructures in, detection of)
IT Algorithm
(for 3-dimensional alignment of protein structures and for detection of
common substructures and structural repeats)
IT Conformation and Conformers
(of proteins, common substructures in, detection of)
IT 60267-61-0, Ubiquitin
RL: ANST (Analytical study)
(3-dimensional substructure in, algorithm for study of)
IT 9026-04-4, Rhodanese
RL: ANST (Analytical study)
(3-dimensional substructures in, algorithm for study of)

=> d his

(FILE 'HOME' ENTERED AT 07:59:48 ON 06 MAY 2003)
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 08:00:00 ON 06 MAY 2003

L1 E TOMIKAWA M/AU
 22 S E3,E12
 L2 E AIKAWA S/AU
 13 S E3,E8,E9
 L3 E MATSUZAWA F/AU
 8 S E4
 E FUJITSU/PA,CS
 L4 E FUJITSU/PA,CS
 23002 S E9-E12
 E JP92-331703/AP,PRN
 E JP92-21012/AP,PRN
 E US6370479/PN
 E US20020072863/PN
 E US20020035434/PN
 E US20020116146/PN
 L5 3 S L1-L3 AND L4
 L6 33 S L1-L3 NOT L5
 SEL DN AN 2
 L7 1 S L6 AND E1-E3
 L8 4 S L5,L7
 L9 3 S L8 NOT 2002/PY

FILE 'WPIX' ENTERED AT 08:08:48 ON 06 MAY 2003

L10 E JP92-331703/AP,PRN
 4 S E4
 L11 E JP92-21012/AP,PRN
 5 S E3,E4
 L12 E US6370479/PN
 1 S E3
 L13 E US20020072863/PN
 1 S E3
 L14 E US20020035434/PN
 1 S E3
 L15 E US20020116146/PN
 1 S E3
 L16 5 S L10-L15
 E TOMIKAWA M/AU
 L17 39 S E3
 E AIKAWA S/AU
 L18 33 S E3
 E MATSUZAWA F/AU
 L19 6 S E3
 E FUJITSU/PA
 L20 126475 S E3
 L21 5 S L16 AND L17-L20
 L22 11 S L17-L19 AND G06F/IC,ICM,ICS
 L23 13 S L17-L19 AND T01/DC
 L24 13 S L17-L19 AND T01-?/MC
 L25 1 S G06T017/IC,ICM,ICS AND L17-L19
 L26 15 S L21-L25
 SEL DN AN 3 4 5 8 9 13 14 15
 L27 7 S L26 NOT E1-E16

FILE 'HCAPLUS' ENTERED AT 08:58:15 ON 06 MAY 2003

FILE 'WPIX' ENTERED AT 08:58:25 ON 06 MAY 2003

L28 8471 S (G06T017 OR G06T015)/IC,ICM,ICS
 L29 10140 S T01-J10C4?/MC
 L30 76679 S (3D OR 3 D OR (THREE OR THIRD) (S) DIMENSION?)/BIX
 L31 82175 S L28-L30
 L32 19028 S L31 AND T01/DC
 L33 33 S L32 AND (ROOT(S) MEAN(S) SQUARE)/BIX
 L34 709 S L32 AND (POINT(S) SET)/BIX

L35 160 S L32 AND (SUBSET OR SUB SET)/BIX
 L36 21 S L34 AND L35
 L37 1 S L33 AND L36
 L38 51 S L33,L36 NOT L27
 L39 31 S L38 AND L33 NOT L27
 L40 4283 S (3 DIMENSION?)/BIX
 L41 529 S L40 AND T01/DC
 L42 8 S L41 AND (ROOT(S)MEAN(S)SQUARE)/BIX
 L43 26 S L41 AND (POINT(S)SET)/BIX
 L44 20 S L41 AND (SUBSET OR SUB SET)/BIX
 L45 47 S L42-L44 NOT L27
 L46 90 S L38,L39,L45
 SEL DN AN 13 22 33 44 70 74 77 85
 L47 8 S L46 AND E17-E34
 L48 16 S L32,L40 AND (SUBGROUP? OR SUB GROUP?)/BIX
 L49 15 S L48 NOT L27,L46
 SEL DN AN 8 9 14
 L50 3 S L49 AND E35-E40
 L51 11 S L47,L50
 L52 84879 S L31,L40
 L53 11 S L52 AND L51
 L54 169 S L52 AND (ROOT(S)SQUAR?)/BIX
 L55 10 S L54 AND (SUBSET? OR SUBGROUP? OR SUB()(SET OR GROUP?))/BIX
 L56 69 S L54 AND SET/BIX
 L57 33 S L54 AND POINT/BIX
 L58 84 S L55-L57
 L59 56 S L58 NOT L27,L46
 L60 26 S L58 NOT L59,L27
 L61 26 S L60 NOT L53
 SEL DN AN 4 9 11
 L62 3 S E41-E49
 L63 84 S L54 NOT L27,L53,L58-L62
 SEL DN AN 14 15 38 50
 L64 4 S E50-E58
 L65 18 S L53,L62,L64 AND L10-L64
 SEL PN APPS L27

 L66 FILE 'DPCI' ENTERED AT 10:06:20 ON 06 MAY 2003
 4 S E59-E79

 FILE 'DPCI' ENTERED AT 10:06:50 ON 06 MAY 2003

 FILE 'WPIX' ENTERED AT 10:07:24 ON 06 MAY 2003
 L67 10 S (US4823306 OR US4853871 OR US4939666 OR US5157736 OR US520091
 L68 6 S (US4747059 OR US5321804 OR US5337402 OR US5704051 OR US570876
 L69 6 S (US4881175 OR US5025388 OR US5058200 OR US5265030 OR US543685
 L70 1 S US6453064/PN
 L71 23 S L67-L70
 L72 22 S L71 NOT L27,L65

 FILE 'WPIX' ENTERED AT 10:14:53 ON 06 MAY 2003

 FILE 'MEDLINE' ENTERED AT 10:15:54 ON 06 MAY 2003
 E VRIEND ?/AU AND GENETICS?/JT AND 1991/PY AND (1 AND 52)/SO
 L73 0 S VRIEND ?/AU AND GENETIC?/JT
 L74 1 S ALEXANDROV ?/AU AND J MOL BIOL?/JT AND 1992/PY
 L75 256 S ORENGO ?/AU
 L76 8 S L75 AND 1992/PY
 L77 1 S L76 AND PROTEINS/JT
 L78 1 S SMITH ?/AU AND MOLVIEW?/TI
 L79 0 S ITAI ?/AU AND 1991/PY AND 10/SO
 L80 0 S ITAI ?/AU AND 1991/PY AND 36/SO
 L81 3 S L74,L77,L78

FILE 'MEDLINE' ENTERED AT 10:20:10 ON 06 MAY 2003

FILE 'HCAPLUS' ENTERED AT 10:21:15 ON 06 MAY 2003

L82	11 S VRIEND ?/AU AND 1991/PY
L83	1 S L82 AND 52/SO
L84	0 S (YAO ? AND SATO ?)/AU AND 1987/PY AND HOMOLOGY/TI
L85	0 S ITAI ?/AU AND 1991/PY AND 36/SO
L86	9 S ITAI ?/AU AND 1987/PY
L87	0 S L86 AND 13/SO